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NEW SOFTWARE PRODUCT

COMPUTATIONAL FLUID DYNAMICS (CFD) WORKSHOP
Combustion Resources, LLC, 1453 West 820 North, Provo, UT 84601.

CFD Workshop is a powerful, low cost tool for performing computational fluid dynamics and combustion simulations on personal computers. It is designed to simplify the application of CFD (CFD for Dummies!). It provides an integrated environment for set-up, solution and visualization of the results. It has a user-friendly interface for quickly generating the computational grid and setting the input and boundary conditions. Run time monitoring shows progress of the solution, including convergence history, mass and energy balances, and plotting of intermediate results. Various plotting capabilities are available for analysis of the results of the simulation.
CFD Workshop runs on PCs with Windows 95/98/NT, making it more accessible to scientists, engineers and students everywhere. It is ideal for use in teaching and classroom environments, and simplifies collaboration between co-workers. It is easy to install, and includes numerous sample problems which simplify getting started with your own problems and applications. It allocates memory dynamically, so problem size is only limited by the amount of memory on your PC.
CFD Workshop uses Automatic Mesh Refinement to improve convergence, assists in establishing grid independence of the solution, and optimizes resource utilization (computer memory and CPU). It consists of separate modules which can be used for analysis of multiphase flow dynamics and combustion, heat transfer, pollutant formation and fouling and slagging. It is based on the comprehensive combustion code, PCGC-3, developed at Brigham Young University's *Advanced Combustion Engineering Research Center* (ACERC) over the last three decades. PCGC-3 has been thoroughly tested and evaluated by comparing predictions with measured results from a variety of facilities ranging from laboratory-scale to full-scale systems.
CFD Workshop is distributed by *Combustion Resources, LLC*, a general engineering company with an emphasis on combustion analysis, testing and simulations. Original developers of PCGC-3 participate in *Combustion Resources*, and provide support and continued development. Consulting services are available through *Combustion Resources* for modeling and testing of combustion systems.
The modular structure of CFD Workshop makes it easier to use by simplifying the user-interface to consist of only the capabilities you specify. The modular structure also makes the memory utilization more efficient. The general characteristics of the modules are:

Basic Module	Heat Transfer Module
Reacting Flow Module	Pollutants Module
Particle Module	Fouling and Slagging Module

System Requirements:	Windows 95/98/NT >200 Mhz (Recommended) 64 MB Memory (>128 MB Recommended) 500 MB Hard Disk Color Monitor
Information and Prices:	Combustion Resources, LLC, 1453 West 820 North, Provo, UT 84601, (801) 225-4356, Fax (801) 226-6276, e-mail: info@combustionresources.com, Internet: www.combustionresources.com

TECHNICAL ABSTRACTS

PASSIVE FLOW CONTROL APPLIED TO A GAS TURBINE BURNER: EFFECT ON COMBUSTION AND FLOW STRUCTURE

C.O. Paschereit and W. Weisenstein, ABB Alstom Technology Ltd., and E. Gutmark, Louisiana State University (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

> Unstable thermoacoustic modes were investigated and controlled in a low emission swirl stabilized experimental burner. Several axisymmetric and helical unstable modes were identified for fully premixed and diffusion type combustion. These unstable modes were associated with flow instabilities related to the wake-like region on the combustor axis due to the inner recirculation zone and shear layer instabilities at the sudden expansion (dump plane). The combustion structure associated with the different unstable modes was visualized by phase locked images of OH chemiluminescence. The axisymmetric mode showed large variation of the heat release during one cycle, while the helical modes showed variations in the radial location of maximal heat release. The axisymmetric mode was the dominant one during unstable combustion. Helical modes could only be obtained when the axisymmetric mode was suppressed by using a non-reflecting boundary condition. Passive control techniques changing the burner geometry were employed to suppress the thermoacoustic pressure oscillations. The different geometrical changes modified the evolution of the inner and outer shear layers, thus affecting the combustion process. The better mixing in the shear layer was documented by water tunnel simulations. With combustion, the unstable heat release became significantly more uniform with low pressure oscillations.

PASSIVE FLOW CONTROL APPLIED TO A GAS TURBINE BURNER: REDUCTION OF EMISSION AND PULSATIONS

E. Gutmark, Louisiana State University, and C.O. Paschereit and W. Weisenstein, ABB Alstom Technology Ltd. (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

> Passive flow control techniques were applied to a low emission swirl stabilized experimental burner which exhibited thermoacoustic instability modes. Several axisymmetric and helical unstable modes were identified for fully premixed and diffusion type combustion. These unstable modes were associated with flow instabilities related to the wake-like region on the combustor axis due to the inner recirculation zone and shear layer instabilities at the sudden expansion (dump plane). Microphones were utilized to monitor the pressure oscillations during the combustion process. The different geometrical changes yielded suppression levels of over 20 dB in the pressure oscillations. In all cases the effect was achieved by modifying the shear layer evolution of the inner and outer recirculation zone, thus affecting the combustion process. The significant reduction in the fluctuating heat release of the flame and the improved mixing due to the passive control methods reduced also the NO_x and CO emissions of the burner.

NUMERICAL SIMULATIONS OF ACOUSTICALLY DRIVEN, BURNING DROPLETS
H.-C. Kim, A.R. Karagozian and O.I. Smith, University of California at Los Angeles (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

The burning characteristics of fuel droplets exposed to external acoustical excitation within a microgravity environment are investigated numerically. The issue of acoustic excitation of flames in microgravity is especially pertinent to understanding the behavior of accidental fires which could occur in spacecraft crew quarters and which could be affected by pressure perturbations as result from ventilation fans or engine vibrations. Combustion of methanol fuel droplets is considered here using a full chemical reaction mechanism. The droplet and surrounding diffusion flame are situated within a cylindrical acoustic waveguide where standing waves are generated with varying frequency and amplitude. Applied pressure levels are limited at present to magnitudes for which the droplet shape remains spherical. A third order accurate, essentially-non-oscillatory numerical scheme is employed to accurately resolve the spatial and temporal evolution of the flame front. Acoustically vs. non-excited external conditions for the burning droplet in microgravity are compared, and the effects of acoustic frequency, sound pressure level, and relative position of the droplet with respect to pressure and velocity nodes are explored.

FLAME STABILITY IN A TRAPPED-VORTEX SPRAY COMBUSTOR
P. Chakka, P.C. Mancilla and S. Acharya, Louisiana State University (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

Flame stabilization mechanisms in a Trapped-Vortex (TV) cavity is investigated experimentally and computationally in the current research. The TV-cavity is placed coaxially in the combustor and the flame is maintained through injection of liquid fuel spray and air from the inside face of the afterbody. This concept was introduced by Roquemore and company of Wright-Patterson AFB for gaseous fuel injection into the cavity and is extended for liquid fuel sprays in the current research. The flame holding capability of the TV-cavity is studied for different equivalence ratios of the secondary injection and overall Lean Blow-Out limits are presented for different primary and secondary flow rates. The interaction and mixing of the main flow with the secondary vortex flow is investigated through the Laser Doppler Velocimetry measurements taken through a quartz window near the cavity. Also, temperature distribution through infrared measurements and pressure fluctuations inside the chamber are presented for complete performance analysis of the TV cavity combustor.

VELOCITY AND THERMAL DISTRIBUTIONS OF AN ACTIVELY CONTROLLED SWIRL-STABILIZED SPRAY FLAME
D. Allgood, S. Acharya and E. Gutmark, Louisiana State University (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

An experimental study of a swirl-stabilized spray flame was performed on a 100 kW model gas turbine combustor. The objective of the research is to investigate the dynamics of the turbulent flowfield and combustion processes for an actively controlled flame with the purpose of enhancing combustion efficiency. The airstream entering the combustor is acoustically excited generating periodic coherent vortical structures in the flowfield. The fuel feed is then modulated at the optimum relative phase instance to provide enhanced fuel and air mixing. The turbulent velocities were measured using a 3 component Aerometrics PDPA system driven by a 6 W argon ion laser. To visualize the thermal characteristics of the flame, a new non-intrusive measurement technique was implemented using an infrared imaging system (Raytheon Radiance HS camera) with a spatial and temporal resolution of 256x256 pixels and 1.2 kHz, respectively. A hyperspectral lens (Pacific Advanced Technology) with the capability of selective wavelength viewing from 3-5 microns was used to image the CO_2 infrared emission wavelength of approximately 4.3 microns. The results from this study will provide insight into the mechanisms involved in the droplet-vortex interactions, the atomization processes, and how active control techniques can be used to enhance the performance of combustors.

CLOSED LOOP CONTROL OF COMBUSTION INSTABILITIES IN A SPRAY COMBUSTION WITH SWIRL

S. Murugappan, S. Acharya and E. Gutmark, Louisiana State University (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

Suppression of thermoacoustic instability was demonstrated in a swirl stabilized spray combustor using closed loop active control system. The inability to completely eliminate the limit cycle and achieve equilibrium stabilization could be attributed to the limited fuel actuator bandwidth. In this situation, the best control requirement is to enforce a stable 'smallest' limit cycle. Generally, the air and/or the fuel are modulated with a phase difference to the resonant frequency of the flow to suppress the oscillations. The method of extremum seeking identifies the optimum phase that needs to be fed to the fuel actuator with respect to the instability frequency to minimize the size of the limit cycle. The present work investigates the features of thermoacoustic oscillation in a swirl stabilized combustor and demonstrates one of the extremum seeking applications. Experiments were performed on a spray combustor with liquid fuel ethanol being injected at the bottom of the combustion cylinder shell through a Parker-Hannifin Research simplex atomizer nozzle. Secondary air was introduced coaxially around the nozzle through two 45-degree swirlers, which provide a swirl number equal to 0.8. The fuel stream was modulated using an automotive fuel injector receiving its signal from a digital signal processor. High sensitivity pressure transducers (Kistler pressure transducer, Model 7061B) and heat flux microsensors (Vatell heat flux microsensor, Model HFM-6D/H) located along the length and circumference of the combustor shell were used to measure the oscillations in the combustor for varying swirl flows, and fuel flow frequencies. Simulations and experiments with the extremum seeking scheme show the potential of controlling the pressure/heat release amplitudes.

OPTICAL DIAGNOSTICS IN THE COMBUSTION CHEMICAL VAPOR DEPOSITION PROCESS

H. Luten, M. Oljaca, T. Tomov and T. Metzger, MicroCoating Technologies, 3839 Green Industrial Way, Chamblee, GA 30341 (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

Optical emission spectroscopy and infrared temperature measurements are used to investigate the structure of a sub-micron droplet spray flame in the Combustion Chemical Vapor Deposition process. The specific system examined in this study is the deposition of barium-strontium-titanate ($Ba_xSr_{1-x}TiO_3$), a high performance ferroelectric. Spectral measurements were used to determine the decomposition rates of the precursors as well as the lifetimes and relative concentrations of the primary decomposition products. The emissions from atomic and unimolecular species reach a maximum value early in the flame and then decrease sharply, indicating very fast reaction rates. This data, however, is a function of the flame temperature. In order to arrive at proper relative concentration data, the optical emission data must be normalized using measured temperature. Two-dimensional temperature maps were obtained using a non-contact, infrared temperature sensor with peak sensitivity at 4.5 microns. It was found that the sodium emission intensity correlates with the flame temperature, and the sodium emission was used as an internal standard for removing the temperature factor and isolating the relative concentration data. While the flame temperature reaches maximum value at approximately 2 cm, the normalized emission for most species reaches peak intensity closer to the nozzle exit.

LASER SPECKLE DISPLACEMENT TECHNIQUE APPLIED TO INSTANTANEOUS TEMPERATURE FIELD MEASUREMENTS OF A FLAME

E. Koc-Alkislar, M.B. Alkislar and L. Lourenco, Fluid Mechanics Research Laboratory FSU/FA&MU (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

The large changes in temperature and composition occurring in flames give rise to rapid refractive index variations. In this study, the temperature distribution of a premixed jet flame is measured in terms of deflections induced by these variations. A cw He-Ne laser serves as a light source. The expanded and collimated laser beam passes through the phase object and deflected light beams are focused on to a ground glass by an imaging lens. The interference from the light scattered by the fine ground glass produces random speckle pattern. For recording of the reference and displaced speckle pattern a Kodak ES-1 CCD camera with a 67 mm zoom lens was focused to a plane away from the ground glass. The camera has the resolution of 1008(H)x1018(V) pixels and it is controlled by a microcomputer, which is capable of acquiring 128 image pairs with a Pentium II CPU at the maximum camera rate of 30 frames/second. The speckle displacement field is computed using a novel mesh-free, second order accurate, processing algorithm. This algorithm is designed to improve the accuracy and spatial resolution of conventional cross-correlation schemes. The high resolution and accuracy also provide higher order approximation to the derivatives of the displacement field. Processing of the displacement field gives the distribution of the density gradient which is integrated over the measurement region to obtain the instantaneous temperature field.

PLANAR LASER INDUCED FLUORESCENCE STUDIES OF LASER INDUCED IGNITION

W. Qin, Y.-L. Chen, C. Parigger and J.W.L. Lewis, The University of Tennessee Space Institute, Tullahoma, TN 37388 (Presented at the *66th Annual Southeastern Section Meeting of the American Physical Society*, Held in Chapel Hill NC, November 1999).

Laser induced breakdown and ignition of atmospheric pressure mixtures of ammonia, oxygen and inert species was studied using planar laser induced fluorescence. The spatial and temporal profiles of the NH and OH radicals were observed following breakdown for a range of mixture fractions. Profiles of non-igniting and igniting mixtures are presented. The gas dynamic and chemical reaction features are shown and compared with computational results.

LASER-SPARK IGNITION COMPUTATIONAL MODELING

I.G. Dors, Y.-L. Chen, J.W.L. Lewis and C. Parigger, The University of Tennessee Space Institute, Tullahoma, TN 37388 (Presented at the *66th Annual Southeastern Section Meeting of the American Physical Society*, Held in Chapel Hill NC, November 1999).

Results are presented of modeling laser-spark ignition processes. Our investigations make use of computational fluid dynamic software from CFD Research Corporation, Huntsville AL, with extensions specific to laser ignition. Of particular interest is

(1) the modeling of laser pulse energy deposition
(2) the inclusion of high temperature (in excess of 20,000 K) effects such as ionization and dissociation of gaseous molecules
(3) the transition from pressure dominated to reaction dominated fluid phenomena, and
(4) comparisons with experimental data sets.

The laser pulse energy deposition is described by asymmetric initial conditions, and the temperature-dependent temporal initiation of multistep, finite-rate reaction models are discussed. Images of the spatio-temporal evolution of the species concentrations and selected maps that describe the flowfield are presented.

PREMIXED EDGE-FLAMES UNDER TRANSVERSE ENTHALPY GRADIENTS
J. Daou and M. Matalon, Northwestern University (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

We describe flame propagation between two opposed reactive streams which may differ in their composition and temperature. Attention is focused on the influence of two non-dimensional parameters: γ, which represents the difference in the enthalpy of the feed streams, and $\in$, which quantifies the ratio between the strain time and a characteristic chemical time. We first present an analysis of the one-dimensional case consisting of two parallel planar flames of unequal strength. Two extinction regimes are identified: for values of γ smaller than a critical value γ^*, the flames extinguish by quenching against each other at the stagnation plane; for $\gamma>\gamma^*$ they extinguish while at a finite distance from each other which increases with γ. We then describe the propagation of two-dimensional flame fronts along the stagnation line. The flame front is thus curved under the combined effect of the flowfield and the transverse enthalpy gradient in the frozen mixture ahead of it; far behind the state of the gas is that of the pair of flat flames introduced above. The problem is studied numerically and complemented by an analytical description corresponding to small values of $\in$. In particular we describe, for different fixed values of γ, the evolution of ignition fronts, characterized by a positive propagation speed, to extinction fronts, characterized by negative speeds, as $\in$ is increased.

FLAME STABILIZATION IN THE FAR FIELD OF A LAMINAR ROUND JET DIFFUSION FLAME
S. Ghosal, Sandia National Laboratories (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

A lifted flame stabilized in the far field of a round laminar jet is considered. Using recent developments in the theory of triple flames, and the Landau-Squire solution for a nonreacting laminar round jet, a transcendental equation is derived for the lift-off height. This equation is shown to have stable solutions if the Schmidt number is greater than unity but no stable solutions if the Schmidt number is less than unity. In the former case, conditions for blowout are obtained.

THE FLOW STRUCTURE OF A PREMIXED JET FLAME CONTROLLED BY COUNTERFLOW
L. Lourenco and E. Koc-Alkislar, Fluid Mechanics Research Laboratory, FSU/FA&MU (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

The nature of the shear layer mixing within the first few jet diameters influences the flame stability. The promising approach to free shear layer control is the exploitation of the inherent instability of the flow to render a global flow response, thereby eliminating the need for externally driven actuators. The global instability of the flow can be accomplished by means of establishing a countercurrent shear layer that is established by the introduction of a reverse flow around the perimeter of an axisymmetric jet at the nozzle exit. A maximum blow-off velocity (U_1) of 42 m/s was achieved at a suction velocity (U_2) of 1.8 m/s. The boundaries of the flame stabilization region were obtained by observing the upper and lower limits of the velocity ratio $R=(U_1-U_2)/(U_1+U_2)$ at a fixed equivalence ratio. The flow structure of the premixed flame was described using the instantaneous velocity and temperature field measurements obtained using PIV and Laser Speckle Displacement techniques. Averaged velocity fields show, that at the presence of counterflow, RMS fluctuation velocity was higher than that of flame without counterflow. This increased velocity fluctuation level was attributed to mixing enhancement. A further testimony for the enhanced mixing was the reduction of mean temperature with the application of suction.

UNSTEADY EXTINCTION BEHAVIOR OF COUNTERFLOW DIFFUSION FLAMES: EXPERIMENTS AND MODELING
V. Santoro, A. Linan and A. Gomez (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

The interaction of a single vortex in gaseous methanol counterflow diffusion flames was studied. The dimensional of the vortices was chosen to minimize curvature effects. Formaldehyde induced fluorescence was used as a complementary marker of the flame, phase-locked LDV was used to measure the instantaneous strain rate on the flame centerline. Under vortex excitation, localized wrinkling in the vicinity of the centerline was observed that, for sufficiently strong vortices, yielded local extinction, with the development of a ‘hole' in the middle of the flame. We observed that the strain rate required for the unsteady extinction proved to be much higher than the ‘quasi-steady' counterpart. A phenomenological explanation will be presented based on the characteristic time scales of the problem. Moreover, a simplified mathematical model will be used to quantify the effects of unsteady strain rates on diffusion flames.

MODEL PREDICTION OF TURBULENT PREMIXED FLAMES FROM THE FLAMELET TO THE THIN REACTION REGIME
S. Menon and V. Sankaran, Georgia Institute of Technology (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

The structure of turbulent premixed flame has many facets in practical combustors due to widely varying turbulence-chemistry interactions that can occur. Premixed combustion in the flamelet, the corrugated flamelet and the distributed reaction (recently called the thin reaction) regimes can coexist within the same device. Models used within large-eddy simulation (LES) methodology to simulate practical systems must therefore be able to predict these space- and time-varying flame structure and propagation characteristics without requiring ad hoc changes. Here, the linear-eddy model (LEM) developed earlier for the flamelet regime has been extended and used to simulate premixed flames over the entire parameter space. A 15-step, 19-species methane/air mechanism has been used in the In-situ Adaptive Tabulation (ISAT) procedure to investigate premixed flame structure from the flamelet to the thin reaction regime without any ad hoc modifications. Qualitative and quantitative comparison with experimental observations show that the LEM is capable of capturing the flame structure in both flamelet and thin reaction regimes. This confirms its viability as a practical model for use within LES.

RESOLUTION REQUIREMENTS FOR SCALAR DISSIPATION MEASUREMENTS IN TURBULENT JETS AND FLAMES
W. Pitts, National Institute of Standards and Technology (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

Scalar dissipation, defined as twice the product of the molecular diffusion coefficient and the local gradient of the mixture fraction dotted with itself, characterizes molecular mixing rates in turbulent flows and has a central role in turbulent combustion modeling. Experimental measurements require sufficient resolution to ensure that the local scalar gradient is effectively constant in time and space. Traditionally, it was argued that it was necessary to resolve spatial features on the order of size of the Batchelor scale, the product of the Kolmogorov scale and the inverse square root of the Schmidt number, which are typically a few hundred micrometers for laboratory flows. More recently, it has been suggested that the required spatial resolution may be 12-25 times larger than the Batchelor scale. Relaxation of the resolution requirements by such large factors would allow measurements with greatly improved signal-to-noise ratios. Unfortunately, recent experiments, including scalar dissipation measurements along a line in an axisymmetric jet of propane into air at the National Institute of Standards and Technology, have shown that the larger estimates for the required spatial resolution will result in partial averaging of the scalar dissipation. Taken together, the studies suggest that in order to fully capture scalar dissipation fluctuations the spatial resolution must be no larger than 2-3 times the Batchelor scale.

THE ROLE OF COMBUSTION IN DIFFUSION FLAME-VORTEX RING INTERACTION

S.-J. Chen and W.J.A. Dahm, The University of Michigan (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

We experimentally investigate flame-vortex interactions as an idealized representation of the coupling between fluid dynamics and combustion in turbulent diffusion flames under conditions that allow the elementary processes to be carefully investigated. Our configuration involves the rollup and burning of an initially flat diffusion flame in a laminar vortex ring formed by impulsively issuing fuel from a round nozzle into an oxidizer environment. Results are obtained under microgravity conditions for propane, ethane, methane fuels, as well as propane diluted with nitrogen, burning in air at atmospheric pressure. With similar ring circulation and fuel volume, the higher sooting propensity of propane rings produced larger radiant losses than the other cases, resulting in a fundamental change in the flame shape. Theoretical fuel consumption time based on simple spherical diffusion flame model agrees well with observed burnout time for most cases. However, trajectories of burning rings do not agree very well with either the inviscid and viscous models of vortex ring translation; effects of heat release must evidently be incorporated through a time varying viscosity. The observations help clarify certain aspects of the coupling between the fluid dynamics and combustion processes in flame-vortex interactions, leading to an improved understanding of turbulent diffusion flames.

NUMERICAL SIMULATION OF A REACTING VORTEX RING USING DETAILED CHEMICAL KINETICS

C. Safta and C.K. Madnia, SUNY-Buffalo (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

A DNS study is conducted to examine the laminar flame-vortex interactions in a reacting vortex ring using ‘realistic' chemical kinetics. The set of equations solved is the compressible multi-species reacting flow equations comprising conservation of mass, linear momentum, energy, and species mass fractions. Transport properties for pure species were evaluated using thermo-molecular databases provided by the Chemkin library. The mixture average formulation was used to evaluate the transport properties for the mixture. Methane combustion was simulated using GRI-Mech v1.2 kinetic model. The vortex ring was generated by a brief discharge of fuel through a round orifice which enters a quiescent ambient with the chemical composition of air. By adjusting the ratio of the ambient and fuel temperatures, the ignition delay time was controlled. The detailed kinetic mechanism will be examined to determine the ignition paths for this unsteady configuration. Time dependent correlations between fundamental parameters such as stoichiometry, heat release rate, hydrodynamic and chemical variables will be investigated to find the most appropriate flame observables for unsteady methane diffusion flames.

POTENTIAL BENEFITS OF USING COUNTERFLOWING SHEAR LAYERS IN PREMIXED COMBUSTION APPLICATIONS

D.J. Forliti, R.D. Gillgrist and P.J. Strykowski, University of Minnesota (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

Linear stability analysis suggests that counterflowing shear layers are more unstable than co-flowing or single stream (jet) shear layers. The instability of counterflowing shear layers can be exploited to control mixing processes. A Particle Image Velocimetry study was conducted to investigate the turbulent characteristics of two mixing configurations: a single stream and a counterflowing shear layer. A 100 percent increase in the turbulence intensity and an increase in the turbulent structure size, for example integral scale, is observed for a moderate level of counterflow. However, an examination of the rms strain rate profiles across the shear layers show comparable levels of peak strain rate. The ability to increase the turbulence intensities and scales without increasing strain would be advantageous in premixed combustion systems, where straining causes a reduction in the turbulent flame speed or may lead to flame quenching.

Differential Diffusion Effects in Turbulent Hydrogen/Oxygen Nonpremixed Flames
T.K. Grimmett and K.K. Nomura, University of California, San Diego (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

The effects of differential diffusion in a turbulent hydrogen/oxygen nonpremixed flame are investigated using direct numerical simulation. A generalized Burke-Schumann formulation that allows for differing species mass and thermal diffusivities as well as finite-rate chemistry is used in the simulations. The formulation is based on a three-step reduced mechanism which assumes partial equilibrium of the two-body chain-carrying reactions yielding an infinitely fast radical-production step, and considers the finite rates of the three-body radical-recombination reactions. This results in a chemical mechanism with H as the only intermediate species. The flowfield is incompressible decaying homogeneous isotropic turbulence (variable density effects are neglected). The initial scalar fields represent reactants which are segregated except for a thin mixed layer where a radical pool is established. The preferential diffusion of the fuel H_2 and intermediate species H are considered. The effects of Damkohler number and nonunity Lewis number on global quantities, conditional averages, and instantaneous values are discussed. Comparisons are made with the limiting case of a single-step, infinite rate reaction.

Fully-Modulated Diffusion Flames
H. Johari, J.C. Hermanson and J.E. Usowicz, Worcester Polytechnic Institute (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

Fully-modulated, turbulent diffusion flames were studied experimentally utilizing ethylene as fuel. A fast solenoid valve was used to fully modulate (completely shut-off) the fuel flow. The fuel was released from a 2 mm nozzle into quiescent, ambient air with injection times ranging from 0.75 to 750 ms. The small nozzle and short injection times are required for future tests of pulsed flames under microgravity conditions. The very short injection times resulted in small injected fuel volumes and compact puffs that burned very rapidly. As the injection time and fuel volume increased, puffs were transformed into elongated flames resembling starting jets. The flame length of elongated pulses were comparable to that of steady flow. In the case of non-interacting compact puffs, the flame length scales linearly with the cube root of the injected volume. When the successive fuel puffs interact due to a fuller duty cycle, the flame length increases in comparison with the individual puffs. The effects of interaction of successive elongated pulses on the flame length were quite small. The effect of Reynolds number on the length of pulsed flames was examined by varying the injection velocity while keeping the injected volume fixed. Over the range of 2000 to 10,000, Reynolds number had only a weak influence on the flame length of non-interacting puffs.

Effects of Heat Release at the Small Scales of Turbulent Flows
J.A. Mullin and W.J.A. Dahm, The University of Michigan (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

Effects of density changes due to heat release by exothermic reactions in turbulent flows are known to alter the outer variable scalings, and thereby affect the resulting entrainment and mixing rates achieved by the flow, even in the absence of any buoyancy effects. There are additional effects of heat release at the small scales of reacting turbulent flows, due among other things to changes in the transport properties of the fluid with temperature, and to the volume source field induced by dilatation. The significance of these heat release effects at the small scales is not known. It is the latter effect that is considered here. We present results from simultaneous PIV and CH PLIF imaging measurements in turbulent jet diffusion flames that resolve the small scales of the flow. Regions of exothermicity as marked by CH concentration fields are compared with those identified by dilatation fields from the PIV measurements. Effects of anisotropy in vector orientations are accounted for, and the resulting comparisons of the velocity gradients induced by the vorticity field and by the dilatation field are obtained. These provide direct insights into the relative significance of dilatation effects in exothermic turbulent reacting flows.

HEAT RELEASE EFFECTS IN NONPREMIXED TURBULENT COMBUSTION

C. Pantano and S. Sarkar, University of California San Diego (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

In high-speed propulsion, density changes due to changes in composition and heat release become important. Direct numerical simulation is used to study the temporally evolving turbulent shear layer with nonpremixed combustion in a methane/air mixture. The effect of heat release on the growth rate of the shear layer and turbulence intensities is addressed. Scalar statistics and conditional averages of the scalar dissipation are also analyzed.

EXAMINATION OF THE ASSUMED BETA PDF SUBGRID-SCALE MODEL FOR NONPREMIXED TURBULENT COMBUSTION WITH HEAT RELEASE

C. Wall, B.J. Boersma and P. Moin, Center for Turbulence Research, Stanford University (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

The assumed beta distribution model for the subgrid-scale probability density function (PDF) of mixture fraction in the large eddy simulation of nonpremixed, turbulent combustion is tested *a priori* for a flow having significant heat release (density ratio of 5). The assumed beta distribution is tested as a model for both the subgrid-scale PDF and the subgrid scale Favre PDF of mixture fraction. The betal model is found to be successful in approximating both types of PDF. To estimate the subgrid-scale variance of mixture fraction, which is required by the beta model, both a scale similarity model and a dynamic model are used. Predictions from the dynamic model are found to be more accurate. Even with the dynamic model, however, the primary limitation of the beta model is found to be the ability to accurately predict subgrid-scale variance.

A SUBGRID SCALE MODEL FOR SCALAR MOMENTS ENCOUNTERED IN TURBULENT COMBUSTION

S. Sarkar and C. Pantano, University of California San Diego, and L. Shao, LMFA, Ecole Centrale, Lyon, France (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

The reaction rate term and radiation heat transfer term in combustion studies involve nonlinear functions of a scalar. Filtering of these nonlinear functions required in large eddy simulations of turbulent combustion leads to unknown subgrid terms. A new model is proposed for the subgrid contribution. The model is found to perform well when predictions of higher moments of the scalar are compared with exact values available from direct simulation of a turbulent shear layer.

LARGE-EDDY SIMULATION OF A TURBULENT PILOTED METHANE/AIR DIFFUSION FLAME

H. Pitsch and H. Steiner, Center for Turbulence Research, Stanford University (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

In the present study, Large-Eddy Simulations for a turbulent, piloted methane/air diffusion flame have been performed and the results are compared to experimental data by Barlow et al. The Smagorinsky model is used to obtain the eddy viscosity, where the Smagorinsky constant is obtained by the Dynamic Model. The Lagrangian Flamelet Model is applied to describe turbulence-chemistry interactions. The model follows a conserved scalar approach, where the resolved mass fractions of chemical species are evaluated using a presumed pdf of the mixture fraction. The pdf is assumed to follow a β-function, depending on the resolved mixture fraction and its subgrid-scale variance, which is also modeled using the Dynamic Procedure. In order to solve the unsteady flamelet equations, the temporal development of the scalar dissipation rate has to be specified from the solution of the turbulent flowfield. In the present model, the conditional average of the scalar dissipation rate as a function of the axial distance from the nozzle is computed from the spatially filtered scalar dissipate rate, which is expressed in terms of the eddy diffusivity and the gradient of the resolved mixture fraction following the model of Girimaji et al.

THE PROGRESS-VARIABLE APPROACH FOR LARGE EDDY SIMULATION OF NON-PREMIXED COMBUSTION

C.D. Pierce and P. Moin, Stanford University (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

A method is proposed for introducing a progress scalar into flamelet models for large eddy simulation of nonpremixed combustion. One-dimensional steady flamelets, which can be inexpensively computed with arbitrarily complex chemistry and multicomponent transport, are parameterized by the progress variable instead of the scalar dissipation rate. Transport equations are solved for both the mixture fraction and the progress variable, where the source term for the progress scalar is determined from the flamelet solutions. This process automatically creates a one-step reduced mechanism based on the flamelet approximation and allows for a better representation of ignition and extinction phenomena. Large eddy simulations, based on the variable density momentum and scalar transport equations with dynamic subgrid-scale models for subgrid stress, scalar flux, and scalar variance, are performed for a piloted, methane/air jet (Sandia Flame D) and a coaxial jet combustor with swirl. Detailed comparisons are made with experimental data.

SOME ISSSUES IN THE USE OF LAMINAR FLAMELET MODEL IN LES SIMULATIONS

X. Cai and F. Ladeinde, Aerospace Research Corp., L.I., P.O. Box 1527, Stony Brook, NY 11790, and B. Sekar, AFRL/PRTC, Wright-Patterson AFB, OH 45433 (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

The usefulness of laminar flamelet model has been well demonstrated by Peters and his co-workers for RANS or κ-ϵ turbulence modeling of pollutant emission and ignition delay for nonpremixed reacting flow. Its extension to large eddy simulations has been reported recently by Cook and Riley. As the input to Cook and Riley's model includes the filtered mixture-fraction variance and dissipation rate, which are unavailable from the traditional LES models, significant efforts have been devoted to model these terms. However, a fundamental quantity of the laminar flamelet theory is the mixture-fraction dissipation rate conditioned on its stoichiometric value, instead of simply the filtered dissipation rate. Hence a connection is required between the conditional and unconditional dissipation rate. Even though counterflow-like structures are scarcely found in turbulent flows, their existence has been assumed in order to provide the required connection. Without using this counterflow assumption, the current work proposes a new model that connects the conditional dissipation rate with the filtered one, using mapping-closure PDF equations. Its performance is discussed, as are the effects on the construction of the model tables in the steady laminar flamelet procedures.

A PDF Method for Turbulent Mixing and Combustion on Three-Dimensional Unstructured Deforming Meshes

D.C. Haworth, Department of Mechanical and Nuclear Engineering, The Pennsylvania State University, and S. Subramaniam, Mechanical & Aerospace Engineering, The State University of New Jersey, Rutgers (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

A hybrid Lagrangian/Eulerian methodology is described for numerical simulation of turbulent mixing and combustion processes in arbitrary three-dimensional geometric configurations. Key numerical issues are addressed including mean estimation and particle/mesh interpolation, particle tracking through unstructured meshes, and particle number density control. The methodology is demonstrated via simulations of turbulent freon/air mixing on an unstructured three-dimensional deforming mesh representing an idealized reciprocating IC engine. Computed profiles of mean and rms freon mole fraction show good quantitative agreement with measurements. Inherent advantages of the Lagrangian/Eulerian pdf approach are demonstrated, compared to Eulerian finite-volume solutions of an equivalent set of moment equations. Preliminary results with heat release are shown. This work broadens the accessibility of PDF methods for practical turbulent combustion systems.

PDF Calculation of Scalar Mixing Layer with Simple Chemical Reactions

T. Kanzaki, Central Research Institute of Electric Power Industry, and S.B. Pope, Cornell University (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

A joint velocity-composition-turbulent frequency PDF(JPDF) model is used to simulate reactive mixing layer in a grid-generated turbulence with the influence of second-order irreversible chemical reactions. To investigate the effects of molecular mixing, a gas flow and a liquid flow are simulated. For a gas flow, the oxidation reaction ($NO+O_3 \rightarrow NO_2+O_2$) between nitric oxide (NO) and ozone (O_3) is used. For a liquid flow, the saponification reaction ($NaOH+HCOOCH_3 \rightarrow HCOONa+CH_3OH$) between sodium hydroxide (NaOH) and methyl formate ($HCOOCH_3$) is used. Both cases are moderately fast reactions. Therefore, reactive scalar statistics are affected by turbulent mixing. The results of calculation are compared with experimental data of Komori et al. (1994) and Bilger et al. (1991).

On the Development of a Flame Wrinkling LES Combustion Model

C. Fureby, FOA Defence Research Establishment, S-17200, Stockholm, Sweden (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

Turbulent combustion is a complex process that affects everyday life. The quest to understand the physical processes is continual and one aspect is the search for improved computational models. A promising approach for simulating turbulent reacting flows of practical interest is Large Eddy Simulation (LES). The philosophy behind LES is to explicitly simulate the large scales of the flow, directly affected by boundary conditions, whilst modeling the smaller scales of the flow. The LES equations are derived by filtering the reacting Navier Stokes equations. The effects of the unresolved eddies appear as additional unknown terms in the LES equations that must be modeled. Subgrid models for non-reacting LES have previously been developed but few extensions to reacting flows have been made since the additional closure problems arising from combustion related terms are difficult to model. This presentation focuses on the development and application of a flame-wrinkling LES combustion model in which transport equations for a reaction coordinate, a modeled flame-wrinkling density and the laminar flame speed are solved. The unresolved transport terms in the momentum and energy equations are not unique to reacting flows and are modeled by a one-equation eddy-viscosity model. A centered second order accurate finite volume based scheme is used to solve the governing equations. The model is here applied to a lean premixed propane/air flame stabilized behind a triangular shaped flameholder. Besides comparing with experimental data a discussion of different modes of combustion found to occur in this combustor will be presented.

LARGE EDDY SIMULATION OF A TURBULENT BUOYANT PLUME
P.E. Desjardin, Sandia National Laboratory (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

Large Eddy Simulations of a helium/air turbulent plume are conducted in order to investigate the buoyancy induced vorticity production mechanisms of this flow. The inlet condition of the plume consists of a low velocity (0.35 m/s) 1 m diameter helium jet emitting upwards into air. This flow configuration is chosen to best match the experimental conditions of the non-reacting helium plume experiments taken at Sandia's FLAME facility. The compressible form of the Favre filtered Navier Stokes, species and energy equations are closed using localized dynamic Smagorinsky subgrid models. Numerical integration is performed using AUSM+ flux vector splitting that employs fifth order upwind biased interpolating stencils and advanced in time using second order Runge-Kutta along with pressure gradient scaling for improved temporal stability. The code uses MPI domain decomposition and is run on Sandia's ASCI red massively parallel computer. Results from the simulations highlight the buoyancy induced vorticity generation and entrainment properties of these flows and the effect of filter width on subgrid modeling. Comparisons to experimental data will be made whenever possible.

EFFECTS OF STRETCH ON CONFINED PREMIXED FLAMES
J.K. Bechtold, New Jersey Institute of Technology, and M. Matalon, Northwestern University (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

The flame speed of a premixed flame is known to depend on curvature and local flow conditions, that is stretch. For thin flames in unconfined environments, both theory and experiment predict a linear relationship between flame speed and stretch, and the sensitivity of this dependence is given in terms of the Markstein number. Here we present some new theoretical predictions regarding stretch effects on premixed flames in enclosed vessels. Specifically, we derive an expression for flame speed in a constant volume vessel. The inherent unsteadiness associated with the increasing pressure gives rise to a more complicated expression for flame speed. We find that flame propagation is strongly influenced by geometry, and the corresponding ‘Markstein numbers' must be interpreted differently from the constant pressure case. We use our model to examine both the planar and spherical geometries, and comparisons are made to recent experimental measurements.

TURBULENCE LENGTH-SCALES IN A FAN-STIRRED COMBUSTION BOMB, MEASURED VIA PARTICLE-IMAGING VELOCIMETRY
V. Sick and M. Hartman, Department of Mechanical Engineering and Applied Mechanics, University of Michigan (Presented at the *52nd Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in New Orleans LA, November 1999).

Combustion experiments are prepared in a fan-stirred reaction bomb that provides internal combustion engine conditions. The experiments aim at the understanding of flame-turbulence interaction. To mimic in-cylinder flow conditions the turbulence properties have to be similar as in engines. The combustion bomb has a near spherical volume of approximately 0.1 m diameter. Turbulence is generated with four fans. Before actual combustion experiments can take place, the turbulence properties as a function of fan speed, that is energy input are studied. A particle-imaging velocimetry setup is used to measure turbulence length scales in the combustion bomb. Air at ambient pressure and temperature is seeded with high temperature dried MgO particles. A double-pulsed Nd:YAG laser at 30 mJ per pulse flash-illuminates a plane of 10 mm height in the center of the bomb. Pulse separation and laser sheet thickness are chosen to guarantee proper detection of the maximum velocities of approximately 10 m/s. A progressive scan ccd camera is used to record the scattering images and data are then processed to yield two-dimensional vector fields. Up to several hundred images per fan speed setting are recorded and mean and rms velocities are computed from these data. An automated routine evaluates the correlation function, which is then used to compute the integral length scale and Taylor scale.

Properties of Electrical Breakdown in Flames

H.S. Uhm, NSWC (Presented at the *41st Annual Meeting of the Division of Plasma Physics of the American Physical Society*, Held in Seattle WA, November 1999).

Properties of electrical discharge in flames and influence of plasma electrons on gas neutrals are investigated by making use of the ionization cross section of air. An analytical expression of air ionization rate is obtained from tabulated data of the ionization cross section of oxygen and nitrogen, and is compared with air ionization rate measured with the applied electric field. The influence of gas temperature on electrical discharge properties is investigated by making use of electron energy-gain in the electric field. Electrical breakdown occurs whenever ionization of neutrals dominates the electron attachment of oxygen molecules. It is found that the breakdown electric field in flames is inversely proportional to the flame temperature T_g, thereby easily generating plasmas in flames. A swarm of low-energy electrons in flames would allow a significant population of electronically excited states of flame molecules to be formed. The analysis shows that the electronic excitation of flame molecules may also considerably reduce the breakdown field. Plasma electrons generate atomic oxygen by the electron attachment of oxygen molecules in high-pressure flames. An example calculation shows that more than 63 percent of oxygen molecules are converted into atoms within 760 μs dwelling time for the plasma with density of n_p=1013 cm^{-3} and temperature of T_e 2.5 eV. Oxygen atoms are the most reactive radicals in flames for material oxidation.

Collisional Deactivation of Ba(5d7p$^3D_1$) by Rare Gases

J. Smedley, S. Coulter, E. Felton and K. Zomlefer, Bates College (Presented at the *Fall Meeting of the New England Section of the American Physical Society*, Held in Colby College, Waterville ME, November 1999).

Collisional deactivation of the (5d7p$^3D_1$) state of Ba by rare gases is studied by time- and wavelength-resolved fluorescence techniques. A pulsed, frequency-doubled dye laser at 273.9 nm excites the (5d7p$^3D_1$) state from the ground state, and fluorescence at 364.1 and 366.6 nm from the (5d7p$^3D_1$-6s5d$^3D_1$) and (5d7p$^3D_1$-6s5d$^3D_2$) transitions, respectively, is monitored in real time at low densities of rare gas to obtain the deactivation rate constants. At 835 K these are:

He = 1.69(±0.08)x$10^{-9}$$cm^3s^{-1}$
Ne = 3.93(±0.14)x10^{-10}
Ar = 4.53(±0.15)x10^{-10}
Kr = 4.64(±0.13)x10^{-10}
Xe = 5.59(±0.22)x10^{-10}

From time-resolved (5d7p$^3D_1$) emission in the absence of rare gas and from the intercepts of the quenching plots, the radiative lifetime of this state is determined to be 100(±1) ns. From wavelength-resolved emission in pure Ba vapor at 364.14 and 366.57 nm, the ratio of A-coefficients for the (5d7p$^3D_1$-6s5d$^3D_1$) and (5d7p$^3D_1$-6s5d$^3D_2$) transitions, respectively is found to be 4(±1). Using time- and wavelength-resolved emission with a low background pressure of rare gas, radiative lifetimes of several near-resonant states are determined from the exponential rise of their fluorescence signals. Integrated fluorescence signals are used to infer the relative cross sections for population transfer from the (5d7p$^3D_1$) state to thirteen near-resonant states.

FORMATION OF LiH BY FAR-WING SCATTERING OF THE Li(2p)+H_2 COMPLEX

S. Bililign and T. Robinson, Department of Physics, North Carolina A&T State University (Presented at the *66th Annual Southeastern Section Meeting of the American Physical Society*, Held in Chapel Hill NC, November 1999).

The interaction of excited alkali atoms with H_2, including both chemical reactions and competitive nonreactive energy transfer are interesting and important processes for study. The simple quasi-one electron nature of the alkali atoms makes detailed theoretical analysis feasible. The high lying states of alkalis are quite hydrogen like. Thus these metal hydrogen systems are useful proving grounds for testing both qualitative theoretical dynamical models and our physical intuition of excited state molecular dynamics. The formation of the LiH from the 2p state is endothermic by greater than 1000 cm^{-1}, thus it appears that at 515 °C, enough of the Li-H_2 collision pairs have sufficient relative energy to make it over the barrier to react and form LiH. Since the reaction proceeds through an endothermic channel, we propose that by scanning to the blue of resonance we can determine a point, at which fluorescence shuts down, indicating energy conversion to form LiH. Preliminary experimental results will be presented.

MULTICONFIGURATION MOLECULAR MECHANICS ALGORITHM FOR POTENTIAL ENERGY SURFACES OF CHEMICAL REACTIONS

Y. Kim, J.C. Corchado, J. Villa, J. Xing and D.G. Truhlar, Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, MN 55455 (to Appear in the *J. Chem. Phys.*).

We present an efficient algorithm for generating semiglobal potential energy surfaces of reactive systems. The method takes as input molecular mechanics force fields for reactants and products and a quadratic expansion of the potential energy surface around a small number of geometries whose locations are determined by an iterative process. These Hessian expansions might come, for example, from ab initio electronic structure calculations, density function theory, or semiempirical molecular orbital theory. A (2x2) electronic diabatic Hamiltonian matrix is constructed from this data such that, by construction, the lowest eigenvalue of this matrix provides a semiglobal approximation to the lowest electronically adiabatic potential energy surface. The theory is illustrated and tested by applications to rate constant calculations for three gas phase test reactions, namely, the isomerization of 1,3-*cis*-pentadiene, $OH+CH_4 \rightarrow H_2O+CH_3$, and $CH_2Cl+CH_3F \rightarrow CH_3Cl+CH_2F$.

TECHNICAL MEETINGS

(Current Additions to this List are Indicated by a Diamond Bullet Marking)

JANUARY 6-8, 2000

4th ISHMT/ASME HEAT AND MASS TRANSFER CONFERENCE
Pune Maharashtta, India.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7284, Fax (212) 705-7143, http://www.asme.org

JANUARY 9-13, 2000

SYMPOSIUM ON ENERGY ENGINEERING IN THE 21st CENTURY
Hong Kong, China.

Information: Ping Cheng, Department of Mechanical Engineering, Hong Kong, University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, (852) 2358-7182, Fax (852) 2358-1543, e-mail: mepcheng@ust.hk, or P. Takahashi, Hawaii Natural Energy Institute, University of Hawaii, Honolulu, HI 96822, (808) 956-8346, Fax (808) 956-2336, e-mail: ptakaha@uhccmvs.uhcc.hawaii.edu

JANUARY 9-13, 2000

PITZER MEMORIAL SYMPOSIUM ON THEORETICAL CHEMISTRY
Berkeley CA.

Information: W.H. Miller, Department of Chemistry, University of California, Berkeley CA 94720, e-mail: pitzer2000@cchem.berkeley.edu

JANUARY 10-13, 2000

38th AIAA AEROSPACE SCIENCES MEETING AND EXHIBIT
Reno NV.

Meeting has Symposia on:
- Aeroacoustics
- Aerodynamic Measurement Technology
- Applied Aerodynamics
- Atmospheric Flight Mechanics
- Microgravity Science and Space Processing
- Plasmadynamics and Lasers
- Propellants and Combustion
- Aerospace Power Systems
- Air-Breathing Propulsion
- Fluid Dynamics
- Intelligent Systems
- Interactive Computer Graphics
- Thermophysics

Information: Meetings Department, American Institute of Aeronautics and Astronautics, 1801 Alexander Bell Drive, Suite 500, Reston, VA 20191, (703) 264-7500 or (800) 639-2422, e-mail: custserv@aiaa.org, http://www.aiaa.org

JANUARY 10-15, 2000

WINTER CONFERENCE ON PLASMA SPECTROCHEM
Fort Lauderdale FL.

Information: R. Barnes, ICP Info Newsletter, P.O. Box 666, Hadley, MA 01003, e-mail: winterconf@chem.umass.edu

JANUARY 22-28, 2000

PHOTONICS WEST
San Jose CA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

FEBRUARY 11-14, 2000

7th LASER APPLICATIONS TO CHEMICAL ANALYSIS MEETING: TOPICAL MEETING OF THE OPTICAL SOCIETY OF AMERICA
Santa Fe NM.

Topics will Include:
- Application of New Laser Sources to Analytical Spectroscopy
- Diode Laser Applications in Combustion, Industrial and Atmospheric Measurements
- Laser Diagnostics for Combustion
- Laser Based Detection Coupled to Microanalytical Separations
- Microoptical Systems for Chemical Analysis
- Laser Based Detection for High Density Chemical Sensing Arrays
- Development and Applications of Single-Molecule Spectroscopy
- Fluorescence Based Methods for Detection of Individual Bimolecules (Including Imaging)

Information: J.B. Jeffries, Molecular Physics Laboratory, SRI International, 333 Ravenswood Ave., Menlo Park, CA 94025, (650) 859-6341, Fax (650) 859-6196, e-mail: Jeffries@crvax.SRI.com, http://www.osa.org/mtg_conf/2000/lacea/
Deadline: Abstracts Due by September 22, 1999.

MARCH 5-8, 2000

8th INTERNATIONAL CONFERENCE ON NUMERICAL COMBUSTION
Amelia Island FL.

Conference Topics Include:
- Turbulence
- Kinetics
- Detonation
- Flames
- Pollution
- Microgravity

- Ignition
- Applications of Parallel Processing
- Tera-scale Computation of Combustion Applications
- Material Synthesis
- Droplets and Sprays
- Heterogeneous Combustion
- Energetic Materials (Propellants and Explosives)
- Engine and Furnace Combustion
- Fires
- Adaptive Numerical Methods
- Software Engineering for Combustion Applications

Invited Speakers Include:

- Premixed Turbulent Combustion: DNS into Modeling, R. Stewart Cant, University of Cambridge, United Kingdom
- Numerical Modeling of Combustion Control in Ramjets, Sergei Frolov, Semenov Institue of Chemical Physics, Russia
- Aerothermochemistry of Flames, Peter Lindstedt, Imperial College, United Kingdom
- Experimental Measurements of Solid Propellant Flame Structure for Model Validation, Timothy Parr, U.S. Naval Air Warfare Center
- Some New Developments in Pre-Mixed Gaseous Combustion, Gregory I. Sivashinsky, Tel Aviv University, Israel
- The Impact of the Accelerated Strategic Computing Initiative on Numerical Combustion, Charles K. Westbrook Lawrence Livermore National Laboratory

Information: Society for Industrial and Applied Mathematics, 3600 University Science Center, Philadelphia, PA 19104, http://www.siam.org/meetings/

MARCH 5-9, 2000

2000 Spring National Meeting of the American Institute of Chemical Engineers on Advanced New Technologies in Industry
Atlanta GA.

Topics will Include:

- 12th Ethylene Producers Conference
- 34th Loss Prevention Conference
- 4th International Conference on Microreaction Technology
- 3rd International Conference on Refining Processes

Information: W.S. Winston Ho, Meeting Program Chair, Department of Chemical and Materials Engineering, 177 Anderson Hall, Lexington, KY 40506, (606) 257-4815, Fax (606) 323-1929, e-mail: wsho@engr.uky.edu

MARCH 6-9, 2000

SAE International Congress and Exposition
Detroit MI.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

♦ MARCH 6-9, 2000

25th INTERNATIONAL TECHNICAL CONFERENCE ON COAL UTILIZATION AND FUEL SYSTEMS
Clearwater FL.

Information: B. Sakkestad, Coal Utilization and Fuel Systems Conference Committee, 104 Edith Drive, Rockville, MD 20850, (301) 294-6080, Fax (301) 294-7480, e-mail: barbarasak@aol.com, web: coaltechnologies.com

♦ MARCH 9-11, 2000

JOINT SPRING MEETING OF THE TEXAS SECTIONS OF THE APS, AAPT AND ZONE 13 OF THE SPS
College Station TX.

Information: R.B. Clark, Department of Physics, Texas A&M University, College Station, TX 77843, (409) 845-3332, Fax (409) 845-2590, e-mail: rbc@tamu.edu, http://www.aps.org/meet/TSS00/

MARCH 12-14, 2000

ASTM COMMITTEE E-13 ON MOLECULAR SPECTROSCOPY
New Orleans LA.

Information: G. Collins, ASTM, (610) 832-9715, Fax (610) 832-9635, e-mail: gcollins@astm.org, http://www.astm.org

MARCH 12-17, 2000

THE PITTSBURGH CONFERENCE, PITTCON 2000
New Orleans LA.

Information: The Pittsburgh Conference, 300 Penn Center Boulevard, Suite 332, Pittsburgh, PA 15235, (412) 825-3220, Fax (412) 825-3224, e-mail: pittconinfo@pittcon.org, http://www.pittcon.org/

MARCH 13-14, 2000

SPRING MEETING OF THE WESTERN STATES SECTION OF THE COMBUSTION INSTITUTE
Colorado School of Mines, Golden CO.

Information: W.J. Pitz, L-353, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551, (925) 422-7730, Fax (925) 422-2644, e-mail: pitz@llnl.gov, http://www.wssci.org/

♦ MARCH 13-14, 2000

DATA FOR SCIENCE AND SOCIETY: 2nd NATIONAL CONFERENCE ON SCIENTIFIC AND TECHNICAL DATA
Washington DC.

Information: P.F. Uhlir, Director, U.S. National Committee for CODATA, National Research Council, Rm. 242, 2101 Constitution Avenue, NW, Washington, DC 20418, (202) 334-2688, Fax (202) 334-2139, e-mail: codataco@nas.edu, http://www.nationalacademies.org/usnc-codata

MARCH 20-24, 2000

MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY
Minneapolis MN.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MARCH 26-30, 2000

SPRING NATIONAL MEETING OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS
Atlanta GA.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 345 East 47th Street, New York, NY 10017, (212) 2705-7338 or (800) 242-4363, http://www.aiche.org

MARCH 26-31, 2000

219th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Francisco CA.

Division of Analytical Chemistry:
- New Frontiers in Analytical Chemistry
- Analytical Problems of the 21st Century
- Limitations of Present Analytical Tools
  T.R. Williams, College of Wooster, Wooster, OH 44691, (330) 263-2115, e-mail: williams@acs.wooster.edu

Division of Fuel Science:
- Fuel Science in the Year 2000: Where Do We Stand, Where Do We Go From Here?
  G.P. Huffman, 533 S. Limestone Street, Suite 111, University of Kentucky, Lexington, KY 40506-0043, (606) 257-4027, Fax (606) 257-7215 e-mail: cffls@pop.uky.edu
- Advances in F-T Chemistry
  B.H. Davis, Center for Applied Energy Research, University of Kentucky, Lexington, KY 40511, (606) 257-0251, Fax (606) 257-0302, e-mail: davis@alpha.caer.uky.edu
- Molecular Modeling of Solid-Fuel Reactions
  L.R. Radovic, Fuel Science Program, Pennsylvania State University, 217 Academic Projects Building, University Park, PA 16802, (814) 863-0594, Fax (814) 865-3075, e-mail: lrr3@psu.edu
- Applications of X-ray and Gamma Ray Techniques in Fuel Science
  K.A. Carrado, CHM/200, 9700 S. Cass Avenue, Argonne National Laboratory, Argonne, IL 60439-4831, (630) 252-7968, Fax (630) 252-9288, e-mail: kcarrado@anl.gov
- Particulate Matter and Fossil Fuel Combustion
  T.J. Feeley III, Department of Energy, Federal Energy Technology Center, P.O. Box 10940, Pittsburgh, PA 15236, (412) 892-6134, Fax (412) 892-5914, e-mail: feeley@fetc.doe.gov
- Solid Fuel Chemistry
  F. Huggins, South Limestone Street, Suite 111, University of Kentucky, Lexington, KY 40506, (606) 257-4045, Fax (606) 257-7215, e-mail: fhuggins@engr.uky.edu

Division of Petroleum Chemistry:
- New Chemistry of Fuel Additives

D. Daly, Fuel Products, Strategic Technology, Lubrizol Co., 29400 Lakeland Blvd., Wickliffe, OH 44092, (440) 943-1200 ext. 4261, Fax (440) 943-9022, e-mail: dtd@lubrizol.com

- CO_2 Conversion and Utilization in Refinery and Chemical Processing
  C. Song, Pennsylvania State University, 209 Academic Projects Building, University Park, PA 16802, (814) 863-4466, Fax (814) 865-3075, e-mail: csong@psu.edu; A.M. Gaffney, DuPont Central R&D, Experimental Station, P.O. Box 80262, Wilmington, DE 19880, (302) 695-1800, Fax (302) 695-8347, e-mail: anne.m.gaffney@usa.dupont.com

Division of Physical Chemistry:

- Physical Chemistry at High Pressure and Temperature
  A.P. Alivisatos, Department of Chemistry, University of California, Berkeley CA 94720, (510) 643-7371, Fax (510) 642-6911, e-mail: alivis@uclink4.berkeley.edu; R. Jeanloz, Department of Geology & Geophysics, University of California, Berkeley CA 94720, (510) 642-2639, Fax (510) 643-9980, e-mail: jeanloz@uclink.berkeley.edu
- Atmospheric Chemistry (Harold Johnston Festschrift)
  C.E. Miller, Department of Chemistry, Haverford College, Haverford, PA 19041, (610) 896-1388, Fax (610) 896-4904, e-mail: cmiller@haverford.edu
- Potential Energy Surfaces: From Polyatomics to Macromolecules
  L.X. Dang, EMSL, Pacific Northwest National Laboratory, P.O. Box 999, Richland, WA 99352, (509) 375-2034, Fax (509) 375-6631, lx_dang@pnl.gov

Information: From the Individual Chairpersons or from Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org
Deadline: 4 Copies of 150-Word Abstract (Original on ACS Abstract Form to Symposium Organizer by November 1, 1999 (Analytical and Physical Chemistry), October 15, 1999 (Fuel and Petroleum Chemistry).

MARCH 26-31, 2000

CORROSION/2000
Orlando FL.

Information: NACE Headquarters, Meetings Department, P.O. Box 218340, Houston, TX 77218, (281) 228-6200, Fax (281) 228-6300, http://www.nace.org

♦ APRIL 3-5, 2000

ROYAL SOCIETY OF CHEMISTRY FARADAY DISCUSSION ON MOLECULAR PHOTOIONIZATION
York UK.

Information: K. Muller-Dethlefs, Department of Chemistry, The University of York, Heslington, York YO10 5DD, UK, 44(0) 1904 434526, Fax 44(0) 1904 434527, e-mail: KMD6@York.ac.uk, http://www.rsc.org/pdf/confs/fara115.pdf

APRIL 3-6, 2000

3rd INTERNATIONAL SYMPOSIUM ON TURBULENCE, HEAT AND MASS TRANSFER
Nagoya, Japan.

Information: T. Tsuji, Symposium Secretary, Department of Mechanical Engineering, Nagoya Institute of Technology, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan, (81) 52-735-5333, Fax (81) 52-735-5359, e-mail: tsuji@heat.mech.nitech.ac.jp, http://heat.mech.nitech.ac.jp/thmt3/

APRIL 3-6, 2000

41st AIAA/ASME/ASCE/AHS/ASC STRUCTURES, STRUCTURAL DYNAMICS AND MATERIALS CONFERENCE
Atlanta GA.

Information: M. Kamat, School of Aerospace Engineering, Georgia Institute of Technology, Atlanta, GA 30332, (404) 894-7439, Fax (404) 894-9313, e-mail: manohar.kamat @aerospace.gatech.edu, or the respective professional society webpages.

APRIL 4-10, 2000

10th INTERNATIONAL CONFERENCE ON HIGH TEMPERATURE MATERIALS CHEMISTRY
Aachen, Germany.

Information: Klaus Hilpert, Forschungszentrum Julich GmbH, Institut fur Werkstoffe der Energietechnik, Julich, Germany D-52425, (49) 2461 613280, Fax (49) 2461 613699, e-mail: k.hilpert@fz-juelich.de

♦ APRIL 7-8, 2000

NEW YORK SECTION SPRING MEETING OF THE AMERICAN PHYSICAL SOCIETY
Corning NY.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

APRIL 8-12, 2000

SPRING TECHNICAL CONFERENCE OF THE ASME INTERNAL COMBUSTION ENGINE DIVISION
San Antonio TX.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

♦ APRIL 10-11, 2000

SPIE's REGIONAL MEETING ON OPTOELECTRONICS, PHOTONICS AND IMAGING: OPTO SOUTHWEST
Albuquerque NM.

Information: B. Peterson, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: bonnie@spie.org, www.spie.org/info/sw/

APRIL 10-14, 2000

10th INTERNATIONAL IUPAC CONFERENCE ON HIGH TEMPERATURE MATERIALS CHEMISTRY
Aachen, Germany.

Topics will Include:

- Synthesis, Properties, and Application of High Temperature Materials
- Vaporization, Molecules, and Clusters
- Interface Processes (Corrosion, Oxidation, Diffusion)

- Technical Processes and Devices at High Temperatures
- Thermodynamic and Kinetic Measurements, Modeling and Databases

Information: K. Hilpert, Forschungszentrum Julich GmbH, Institut fur Werkstoffe der Energietechnick (IWE 1), 52425 Julich, Germany, (49) 2461 61 3280, Fax (49) 2461 61 3699, e-mail: k.hilpert@fz-juelich.de, http://www.fz-juelich.de/oea/termine.html

APRIL 10-14, 2000

3rd INTERNATIONAL SEMINAR IN FIRE AND EXPLOSION HAZARDS
Lake Windermere, UK.

Information: G. Makhviladze, Centre for Research in Fire and Explosion Studies, University of Central Lancashire, Preston PR1 2HE, UK, (01772) 893222, Fax (01772) 892916, e-mail: g.makhviladze@uclan.ac.uk, http://www.uclan.ac.uk/commerc/fire.htm

APRIL 11-13, 2000

GASIFICATION FOR THE FUTURE
Noordwijk, The Netherlands.

Information: J. Black, IChemE's Conference Department, 165-189 Railway Terrace, Rugby, Warwickshire CV21 3HQ, UK, (44) 1788-578214, Fax (44) 1788-577182, e-mail: jblack@icheme.org.uk

APRIL 11-14, 2000

5th EUROPEAN CONFERENCE ON INDUSTRIAL FURNACES AND BOILERS
Porto, Portugal.

Information: INFUB c/o Albino Reis, Rua Gago Coutino, 185-187, 4435 Rio Tinto, Portugal, (2) 9734624/9730747, Fax (2) 9730746, e-mail: conference@infub.pt, http://www.infub.pt

APRIL 12-14, 2000

3C STEREO AND HOLOGRAPHIC PIV APPLICATION TO TURBULENCE MEASUREMENTS: EUROMECH COLLOQUIUM 411
Rouen, France.

Information: M. Trinite, CORIA-UMR 6614, Universite et INSA de Rouen, F-76821 Mont Saint Aignan Cedex, France, (33) 2-35-14-65-58, Fax (33) 2-35-70-83-84, e-mail: trinite@coria.fr

♦ APRIL 14-15, 2000

NEW ENGLAND SECTION SPRING MEETING OF THE AMERICAN PHYSICAL SOCIETY
Providence RI.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

APRIL 16-18, 2000

SPRING TECHNICAL MEETING OF THE CENTRAL STATES SECTION OF THE COMBUSTION INSTITUTE
Indianapolis IN.

Invited Papers Include:

- The Real Sequence of Processes to be Modeled in Diesel Engine Combustion
  P.F. Flynn, Cummins Engine Co., Inc.
- A Current Perspective on In-Cylinder Turbulent Thermal-Fluids Processes in Spark Ignited Reciprocating IC Engines
  D. Haworth, Pennsylvania State University
- Multidimensional Modeling of Reacting Flow in Stationary Combustors
  W.A. Fiveland, Combustion Engineering, Inc.
- Modeling of Gas-Turbine Combustors
  M.S. Anand, Rolls Royce Allison

Information: D.L. Reuss, General Motors R&D, 30500 Mound Road, Warren, MI 48090, (810) 986-0887, Fax (810) 986-0176, e-mail: dreuss@gmr.com
Deadline: Submit Abstract by January 4, 2000, 6-Page Paper by March 1, 2000. Abstracts of Poster Presentations by February 15, 2000.

APRIL 24-28, 2000

MATERIALS RESEARCH SOCIETY SPRING MEETING
San Francisco CA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (412) 779-3003, e-mail: info@mrs.org

APRIL 26-30, 2000

2nd INTERNATIONAL CONFERENCE ON ATOMIC AND MOLECULAR DATA AND THEIR APPLICATIONS
Oxford UK.

Information: K. Berrington, e-mail: k.berrington@shu.ac.uk, http://physics.nist.gov/icamdata

APRIL 29-MAY 1, 2000

ANNUAL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Long Beach CA.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ MAY 2-4, 2000

HALON OPTIONS TECHNICAL WORKING CONFERENCE
Albuquerque NM.

Information: L. Oliver, The University of New Mexico, 901 University Boulevard SE, Albuquerque, NM 87106, (505) 272-7250, Fax (505) 272-7203, e-mail: oliver@nmeri.unm.edu

MAY 7-12, 2000

CLEO/QELS 2000
San Francisco CA.

Information: Meetings Department, American Physical Society, One Physics Ellipse, College Park, MD 20740, (301) 209-3286, http://www.osa.org/mtg_conf, http://physics.wm.edu/~cooke/dis/dis.html

MAY 8-11, 2000

ASME TURBO EXPO: LAND, SEA AND AIR
Munich, Germany.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (404) 847-0072 or (212) 591-7008, Fax (212) 705-7143, http://www.asme.org

MAY 8-11, 2000

UNITED ENGINEERING CONFERENCE ON THE EFFECTS OF COAL QUALITY ON POWER PLANT PERFORMANCE: ASH PROBLEMS, MANAGEMENT AND SOLUTIONS
Park City UT.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, e-mail: engfnd@aol.com, http://www.engfnd.org/engfnd/conf.html

♦ MAY 8-12, 2000

INTERNATIONAL CONFERENCE ON INCINERATION AND THERMAL TREATMENT TECHNOLOGIES
Portland OR.

Information: L.B. Cohen, University of California, EH&S, 300 University Tower, Irvine CA 92697, (949) 824-5859, Fax (949) 824-1900, e-mail: lbarnow@uci.edu

♦ MAY 9-11, 2000

5th INTERNATIONAL CONFERENCE ON COAL UTILIZATION SCIENCE AND TECHNOLOGY
Budapest, Hungary.

Information: Z. Katona, Department of Energy, Technical University of Budapest, 1111 Budapest, Muegyetem rkp. 3, Hungary, Fax (1) 463-3273, or in the UK, J. Tucker, 44(0) 1242-763361.

MAY 14-19, 2000

197th MEETING OF THE ELECTROCHEMICAL SOCIETY
Toronto, Ontario, Canada.

Topics Include:
- General Session on Corrosion
- Plasma Processing

- 15th International Conference on Chemical Vapor Deposition
- Sensors for Energy Technologies

Information: http://www.electrochem.org/meetings

MAY 16-19, 2000

33rd MIDDLE ATLANTIC REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Newark DE.

Information: G.L. Trainor, DuPont Pharmaceuticals Co., P.O. Box 80353, Wilmington, DE 19880, (302) 695-3580, Fax (302) 695-8344, e-mail: trainogl@carbon.dmpc.com

♦ MAY 17-18, 2000

CONFERENCE ON SELECTIVE CATALYTIC AND NONCATALYTIC REDUCTION FOR NO_x CONTROL
Pittsburgh PA.

Information: K. Lockhart, FETC Conference Services, 626 Cochrans Mill Road, P.O. Box 10940, MS 922-178C, Pittsburgh, PA 15236, (412) 386-4763, Fax (412) 386-6486, e-mail: lockhart@fetc.doe.gov

MAY 17-19, 2000

32nd CENTRAL REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Covington KY.

Information: R. D'Alonzo, Procter & Gamble, Sharon Woods Technical Center, 11450 Grooms Road, Cincinnati, OH 45242, (513) 626-1977, Fax (513) 626-5145, e-mail: dalonzorp@pg.com

♦ MAY 19-20, 2000

NORTHWEST SECTION MEETING OF THE AMERICAN PHYSICAL SOCIETY
Eugene OR.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MAY 22-26, 2000

4th MINSK INTERNATIONAL HEAT AND MASS TRANSFER FORUM
Minsk, Belarus.

Information: I. Gurevich, Secretary of the MIF-IV Organizing Committee, A.V. Luikov Heat and Mass Transfer Institute, National Academy of Sciences of Belarus, 15, P. Brovka St., Minsk, 220072, Belarus, (375) 17.284-21-36, Fax (375) 17.232-25-13, e-mail: igur@hmti.ac.by, http://www.itmo.by/forum/forum7/index.html

JUNE 4-7, 2000

32nd GREAT LAKES REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Fargo ND.

Information: G.J. McCarthy, North Dakota State University, Department of Chemistry, Ladd Hall 104B, Fargo, ND 58105, (701) 231-7193, Fax (701) 231-8883, e-mail: gmccarth@prarie.nodak.edu

JUNE 4-8, 2000

TURN OF THE CENTURY IN ATOMIC SPECTROMETRY AND ELEMENT ANALYSIS: PAST, PRESENT AND FUTURE
Interlaken, Switzerland.

Information: G. Vujicic, SASP c/o IWM, Industriestr. 59, Glattbrugg, Switzerland CH-8152, (41) (0) 1 810 57 72, Fax (41) (0) 1 810 09 78, e-mail: gvujicic@swissonline.ch, http://www.sasp.ch/

JUNE 8-10, 2000

JOINT 55th NORTHWEST/16th ROCKY MOUNTAIN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Idaho Falls ID.

Information: E.G. Meyer, 214 Arts & Sciences, University of Wyoming, Laramie, WY 82071, (307) 766-5445.

♦ JUNE 11-12, 2000

16th WORLD PETROLEUM CONGRESS
Calgary, Alberta, Canada

Information: 16th World Petroleum Congress, 1350, 144-4 Avenue SW, Calgary, Alberta, Canada T2P 3N4, (403) 218-2000, Fax (403) 218-2002, e-mail: cdn.assoc@wpc2000.com, web: www.wpc2000.com

♦ JUNE 11-14, 2000

ASME/ZSITS INTERNATIONAL THERMAL SCIENCE SEMINAR
Bled, Slovenia.

Information: I. Golobic, Faculty of Mechanical Engineering, University of Ljubljana, Askerceva 6, 1000 Ljubljana, Slovenia, (386) 61-1771420, Fax (386) 61-218567, e-mail: iztok.golobic@uni-lj.si, or A.E. Bergles, 180 River View Lane, Centerville, MA 02632, Phone/Fax (508) 790-4873, e-mail: abergles@aol.com, http://www.ltt.uni-lj.si/itss2000/

JUNE 11-15, 2000

SUMMER MEETING OF THE ASME FLUIDS ENGINEERING DIVISION
Boston MA.

Symposia will Include:

- Flows in Manufacturing Processes
- Numerical Developments in CFD
- Non-Invasive Measurements in Multiphase Flow
- Advances in Numerical Modeling of Aerodynamics and Hydrodynamics in Turbomachinery
- Erosion Processes
- Fluid Flow in Microsystems: Measurement, Analysis, and Applications
- Numerical Methods for Multiphase Flows
- Experimental and Numerical Flow Visualization and Laser Anemometry

Forums will be Held on the Following Topics:

- Finite Element Applications in Fluid Dynamics
- Turbulent Flows
- Laminar Flows
- High Speed Jet Flows
- Advances in Fluids Engineering Education
- CFD Applications in Automotive Flows
- Bifurcation, Instability, and Hysteresis in Fluid Flow
- Three-Dimensional Flows
- CFD Applications in Large Facilities
- Open Forum on Multiphase Flows
- Submicron Particle Flows
- Fluid Measurements and Instrumentation
- Fluid Machinery Forum
- Advances in Free Surface and Interface Fluid Dynamics
- Simulation of the Interaction of Transportation Vehicles with the Environment
- Forum on Developments in CFD Code Verification and Validation
- Cavitation and Multiphase Flow Forum

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

JUNE 11-15, 2000

48th ASMS CONFERENCE ON MASS SPECTROMETRY AND ALLIED TOPICS
Long Beach CA.

Information: http://www.asms.org

♦ JUNE 12-16, 2000

55th SYMPOSIUM ON MOLECULAR SPECTROSCOPY
Columbus OH.

Information: T.A. Miller, International Symposium on Molecular Spectroscopy, Department of Chemistry, The Ohio State University, 120 West 18th Avenue, Columbus, OH 43210.

JUNE 14-17, 2000

DIVISION OF ATOMIC, MOLECULAR AND OPTICAL PHYSICS OF THE AMERICAN PHYSICAL SOCIETY
Storrs CT.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ JUNE 15-17, 2000

JOINT 55th ACS NORTHWEST/16th ROCKY MOUNTAIN REGIONAL MEETING
Idaho Falls ID.

Information: E.G. Meyer or D. Nelson, 214 Arts & Sciences, University of Wyoming, Laramie, WY 82071, (307) 766-5445, Fax (307) 766-2697, e-mail: egmeyer@uwyo.edu or danelson@wyoming.com; T. Allen or F. Stewart, INEEL, P.O. Box 1625, MS 2008, Idaho Falls, ID 83415, (208) 526-8594, Fax (208) 526-8541, e-mail: fsf@inel.gov, web site: http:/www2.ida.net/acsid/norm2000/

JUNE 18-21, 2000

29th NORTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Storrs CT.

Information: G. Epling, University of Connecticut, 215 Glenbrook Road, Storrs, CT 06269, (860) 486-3214, Fax (860) 486-2981, e-mail: epling@nucleus.chem.uconn.edu

JUNE 18-22, 2000

ANNUAL MEETING OF THE AIR AND WASTE MANAGEMENT ASSOCIATION
Salt Lake City UT.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org

JUNE 18-23, 2000

OPTICS IN COMPUTING
Quebec City, Quebec, Canada.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

JUNE 19-20, 2000

CEC/SAE FUELS AND LUBRICANTS SPRING MEETING AND EXPOSITION
Le Palais des Congress, Paris, France.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

JUNE 19-22, 2000

21st AIAA ADVANCED MEASUREMENT TECHNOLOGY AND GROUND TESTING CONFERENCE: FLUIDS 2000 AND EXHIBIT: 31st AIAA PLASMADYNAMICS AND LASERS CONFERENCE: 34th AIAA THERMOPHYSICS CONFERENCE
Denver CO.

Information: J.A. Morrow, Department of Aeronautics, United States Air Force Academy, 2354 Fairchild Drive, #6H22, U.S. Air Force Academy, CO 80840, (719) 333-3434, Fax (719) 333-4813, e-mail: MorrowJA.dfan@usafa.af.mil, or http://www.aiaa.org

♦ JUNE 21-23, 2000

60th PHYSICAL ELECTRONICS CONFERENCE
Baton Rouge LA.

Information: R.L. Kurtz, Department of Physics and Astronomy, 202 Nicholson Hall, Louisiana State University, Baton Rouge, LA 70803, (225) 388-4028, Fax (225) 388-5855, http://www.physicalelectronics.org/

♦ JUNE 26-30, 2000

INTERNATIONAL WORKSHOP ON UNSTEADY COMBUSTION AND INTERIOR BALLISTICS
St. Petersburg, Russia.

Information: V. Babuk, e-mail: kaf-m1@bstu.spb.su, or babuk@peterlink.ru

JULY 1-7, 2000

WORLDWIDE RENEWABLE ENERGY CONGRESS
Brighton UK.

Information: A. Sayrigh, 147 Hilmanton, Lower Earley, Reading RG6 4HN, UK.

♦ JULY 9-14, 2000

6th POLISH CONFERENCE ON ANALYTICAL CHEMISTRY
Gliwice, Poland.

Information: 6th Polish Conference on Analytical Chemistry, Department of Analytical and General Chemistry, Silesian Technical University, ul. M. Strzody 9, 44-100 Gliwice, Poland, phone/fax 48-32-237-12-05, e-mail: analityk@zeus.polsl.gliwice.pl, http://www.polsl.gliwice.pl/~analityk

♦ JULY 10-13, 2000

10th INTERNATIONAL SYMPOSIUM ON APPLICATIONS OF LASER TECHNIQUES TO FLUID MECHANICS
Lisbon, Portugal.

Information: M.V. Heitor, Department of Mechanical Engineering, Instituto Superior Tecnico, Av. Rovisco Pais, 1049-001 Lisboa, Portugal, (351) 1-841-7379/7732, Fax (351) 1-849-6156, e-mail: llaser@in3dem.ist.utl.pt, http://in3.dem.ist.utl.pt/lisboa-laser

JULY 16-19, 2000

36th AIAA/ASME/SAE/ASEE JOINT PROPULSION CONFERENCE AND EXHIBIT ON PROPULSION: THE KEY TO EXPLORING NEW WORLDS
Huntsville AL.

Information: B. Noblitt, Conference General Chair, TRW, Suite 1231, 303 Williams Avenue, Huntsville, AL 35801, (256) 533-3714, Fax (256) 533-0137, e-mail: bobby.noblitt@trw.com, or http://www.aiaa.org/calendar

♦ JULY 16-20, 2000

8th INTERNATIONAL CONFERENCE ON LIQUID ATOMIZATION AND SPRAY SYSTEMS
Pasadena CA.

Information: D. Talley, USAF Research Laboratory, AFRL/PRSA, 10 East Saturn Boulevard, Edwards AFB, CA 93524, (661) 275-6174, Fax (661) 275-6245, e-mail: douglas_talley@ple.af.mil, http://www.iclass2000.uci.edu/

♦ JULY 17-20, 2000

10th BIENNIAL NATIONAL ATOMIC SPECTROSCOPY SYMPOSIUM OF THE ROYAL SOCIETY OF CHEMISTRY
Sheffield, UK.

Information: P. Krause, Centre for Analytical Science, Dainton Building, Brookhill, Sheffield, S3 7HF, UK, 44(0) 114-222-3652, Fax 44(0) 114-222-3650, e-mail: p.krause@sheffield.ac.uk, http://www.rsc.org/lap/rsccom/dab/ana002.htm

♦ JULY 22-27, 2000

18th SYMPOSIUM ON PHOTOCHEMISTRY: PHOTOCHEMISTRY INTO THE NEW CENTURY
Dresden, Germany.

Information: S.E. Braslavsky, Max-Planck Institut fur Strahlenchemie, Postfach 101365, D-45413 Mulheim an der Ruhr, Germany, (49) 208-306-3681, Fax (49) 208-306-3951, e-mail: braslavskys@mpi-muelheim.mpg.de, http://www.chm.tu-dresden.de/photo/iupac2000/

JULY 23-26, 2000

ASME INTERNATIONAL JOINT POWER GENERATION CONFERENCE AND EXPOSITION
Miami Beach FL.

Information: N.A. Moussa, BlazeTech Corporation, 24 Thorndike Street, Cambridge, MA 02141, (617) 661-0700, Fax (617) 661-9242, amoussa@blazetech.com, or http://www.asme.org/conf/

♦ JULY 23-27, 2000

16th INTERNATIONAL SYMPOSIUM ON GAS KINETICS
Cambridge UK.

Information: G. Southwell, Secretary to the 16th International Symposium on Gas Kinetics, University Chemical Laboratory, Lensfield Road, Cambridge, CB2 1EW, England, Fax (1223) 336362, http://www.gk2.ch.cam.ac.uk

JULY 23-28, 2000

ENERGEX 2000: 8th INTERNATIONAL ENERGY FORUM
Las Vegas NV.

Topics will Include:
- Renewable Energies
- Clean Coal Technologies
- Fossil Fuels
- Energy and Economics
- Climatic Change
- International Law
- General Topics
- International Reports
- Nuclear Energy
- Architecture

Information: P. Catania, Faculty of Engineering, University of Regina, Regina, SK S4S 0A2, Canada, (306) 585-4363, Fax (306) 585-4855, e-mail: peter.catania@uregina.ca, http://www2.regina.ism.ca/ief/index/htm or http://www.energysource.com/ief/updates/

JULY 24-28, 2000

35th INTERSOCIETY ENERGY CONVERSION ENGINEERING CONFERENCE
Las Vegas NV.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7008, Fax (212) 705-7143, http://www.asme.org

JULY 30-AUGUST 4, 2000

SPIE ANNUAL MEETING
San Diego CA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

JULY 30-AUGUST 4, 2000

28th INTERNATIONAL SYMPOSIUM ON COMBUSTION
Edinburgh, Scotland.

Information: S.S. Terpack, The Combustion Institute, 5001 Baum Boulevard, Suite 635, Pittsburgh, PA 15212, (412) 687-1366, Fax (412) 687-0340, e-mail: combust@telerama.lm.com

AUGUST 1-5, 2000

35th IECEC INTERSOCIETY ENERGY CONVERSION ENGINEERING CONFERENCE
Las Vegas NV.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7008, Fax (212) 705-7143, http://www.asme.org

♦ AUGUST 6-11, 2000

15th INTERNATIONAL CONFERENCE ON NUCLEATION AND ATMOSPHERIC AEROSOLS
Rolla MO.

Information: B. Hale, University of Missouri, 205 Physics, Rolla, MO 65409, (573) 341-4795, e-mail: bhale@umr.edu or marrku.kulmala@helsinki.fi, http://www.umr.edu/~icnaa

♦ AUGUST 6-11, 2000

16th IUPAC CONFERENCE ON CHEMICAL THERMODYNAMICS
Halifax, Nova Scotia, Canada.

Information: M.A. White, Department of Chemistry, Dalhousie University, Halifax, Nova Scotia B3H 4J3, Canada, (902) 494-3894, Fax (902) 494-1310, e-mail: mary.anne.white@dal.ca, http://IS.DAL.CA/~ICCT

♦ AUGUST 8-12, 2000

8th INTERNATIONAL CONFERENCE ON ELECTRONIC SPECTROSCOPY AND STRUCTURE
Berkeley CA.

Information: ICESS8, Advanced Light Source, Lawrence Berkeley National Laboratory, MS 6-2100, Berkeley, CA 94720, Fax (510) 486-4773, e-mail: icess@lbl.gov, http://www-als.lbl.gov/icess

♦ AUGUST 13-16, 2000

5th INTERNATIONAL CONFERENCE ON GREENHOUSE GAS TECHNOLOGIES
Cairns, Queensland, Australia.

Information: GHGT-5 Secretariat, C. Paulson, CSIRO Energy Technology, PO Box 136, North Ryde, NSW 1670, Australia, (2) 9490-8790, Fax (2) 9490-8819, e-mail: c.paulson@det.csiro.au

AUGUST 13-18, 2000

TURBINE 2000, INTERNATIONAL SYMPOSIUM ON HEAT TRANSFER IN GAS TURBINE SYSTEMS
Izmir, Turkey.

Information: R.J. Goldstein, Conference Chair, Department of Mechanical Engineering, University of Minnesota, Minneapolis, MN 55455, (612) 625-5552, Fax (612) 625-3434, e-mail: rjgumn@mailbox.mail.umn.edu, http://ichmt.me.metu.edu.tr
Deadline: Abstracts Due by February 29, 2000.

AUGUST 14-17, 2000

18th AIAA APPLIED AERODYNAMICS CONFERENCE
Denver CO.

Information: N.E. Suhs, Applied Aerodynamic Technical Program Chair, Naval Air Systems Command, Building 2187, Unit 5, Suite 1390A, 48110 Shaw Road, Patuxent River, MD 20670, (301) 342-0311, Fax (301) 342-8585, e-mail: suhsne@navair.navy.mil, or http://www.aiaa.org/calendar
Deadline: Abstract by January 3, 2000

♦ AUGUST 14-18, 2000

12th INTERNATIONAL CONGRESS ON THERMAL ANALYSIS AND CALORIMETRY
Copenhagen, Denmark.

Information: O.T. Sorensen, Materials Research Department, Riso National Laboratory, DK-4000 Roskilde, Denmark, 45-4677-5800, Fax 45-4677-5758, e-mail: o.toft.sorensen@risoe.dk, http://www.risoe.dk/ictac

♦ AUGUST 16-22, 2000

JAHN TELLER SYMPOSIUM
Boston MA.

Information: M. Kaplan, Simmons College and Boston University, (617) 521-2727, e-mail: kaplan@buphy.bu.edu, or G. Zimmerman, Boston University, (617) 353-2189, e-mail: goz@buphy.bu.edu

AUGUST 20-22, 2000

34th ASME NATIONAL HEAT TRANSFER CONFERENCE
Pittsburgh PA.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7795, Fax (212) 705-7143, http://www.asme.org

AUGUST 20-24, 2000

220th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Washington DC.

Division of Fuel Chemistry:

- 1990 Clean Air Act Amendments: A 10-Year Assessment
  J.J. Helble, University of Connecticut, Department of Chemical Engineering, U-222, Storrs, CT 06269, (860) 486-4602, Fax (860) 486-2959, e-mail: helble@eng2.uconn.edu
- Inorganics in Fossil Fuels, Waste Materials, and Biomass: Characterization, Combustion Behavior, and Environmental Issues
  C.L. Senior, Physical Sciences, Inc., 20 New England Business Center, Andover, MA 01810, (978) 689-0003, Fax (978) 689-3232, e-mail: senior@psicorp.com
- Waste Material Recycling for Energy and Other Applications
  S.V. Pisupati, Fuel Science Program, Pennsylvania State University, 404 Academic Projects Building, University Park, PA 16802, (814) 865-0874, Fax (814) 863-8892, e-mail: sxp17@psu.edu

- Fossil Fuels and Global Climate/CO_2 Abatement
  R. Warzinski, USDOE/FETC, Box 10940, Building 83-324, Pittsburgh, PA 15236, (412) 892-5863, e-mail: warzinsk@fetc.doe.gov
- Production of Fuels and Chemicals from Synthesis Gas
  D.B. Dadyburjor, Department of Chemical Engineering, P.O. Box 6102, West Virginia University, Morgantown, WV 26506, (304) 293-2111 ext 2411, Fax (304) 293-4139, e-mail: dadyburjor@cemr.wvu.edu
- Solid Fuel Chemistry
- Chemistry of Liquid and Gaseous Fuels
  F. Huggins, South Limestone St., Suite 111, University of Kentucky, Lexington, KY 40506, (606) 257-4045, Fax (606) 257-7215, e-mail: fhuggins@engr.uky.edu

Division of Petroleum Chemistry:

- Emission Control in Petroleum Processing
  P. O'Connor, U.S. Ozkan, Department of Chemical Engineering, Ohio State University, 140 W. 19th Avenue, Columbus, OH 43210, (614) 292-6623, Fax (614) 292-3769, e-mail: ozkan.1@osu.edu
- Structure of Jet Fuels VI
  W.E. Harrison, Department of the Air Force, WL/POSF, Building 490, Area B, 1790 Loop Road N., Wright-Patterson AFB, OH 45433, (937) 255-6601, Fax (937) 255-1125, e-mail: harriswe@wl.pafb.af.mil

Division of Physical Chemistry:

- Chemistry Under Extreme Conditions
  R. Morris, AFRL/VSBP, 29 Randolph Rd., Hanscom AFB, MA 01731, (781) 377-8758, Fax (781) 377-5088, e-mail: morris@plh.af.mil
- Very Low Temperature Spectroscopy and Dynamics
  W. Stwalley, Department of Physics, University of Connecticut, 2152 Hillside Road, Storrs, CT 06269, (860) 486-4924, Fax (860) 486-3346, e-mail: stwalley@uconnvm.uconn.edu

Information: From the Individual Chairpersons or from the Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

♦ AUGUST 20-25, 2000

17th International Conference on Raman Spectroscopy
Beijing, China.

Information: Shu-Lin Zhang, President of ICORS 2000, e-mail: icors@pku.edu.cn, http://icors.pku.edu.cn

AUGUST 22-25, 2000

9th International (Millennium) Symposium on Flow Visualization
Edinburgh, Scotland.

Information: I. Grant, Heriot-Watt University, Edinburgh, Scotland, EH10 5PJ, UK, (44) 1314478800, Fax (44) 1314478660, e-mail: 9misfv@ode-web.demon.co.uk, Web Site: http://www.ode-web.demon.co.uk/9misfv
Deadline: Abstract Template should be Downloaded from the Web. 4 Pages or Less to be Submitted by December 12, 1999. Final Manuscripts Due May 15, 2000.

AUGUST 26-30, 2000

15th EUROPHYSICS CONFERENCE ON ATOMIC AND MOLECULAR PHYSICS OF IONIZED GASES
Miskolc-Lillafured, Hungary.

Information: Z. Donko, c/o Eotvos Lorand Physical Society, H-1371 Budapest, P.O. Box 433, Hungary, e-mail: escampig@elft.mtesz.hu, http://elft.mtesz.hu/escampig2000

♦ AUGUST 27-31, 2000

14th INTERNATIONAL CONGRESS OF CHEMICAL AND PROCESS ENGINEERING
Prague, Czech Republic.

Information: CHISA 2000, Novotneho Lavka 5, 116 68 Praha 1, Czech Republic, (420) 2-2108-2333, Fax (420) 2-2108-2336, e-mail: chisa@csvts.cz, http://www.chisa.cz

AUGUST 27-SEPTEMBER 1, 2000

25th EUROPEAN CONGRESS ON MOLECULAR SPECTROSCOPY
Coimbra, Portugal.

Information: R. Fausto, Department of Chemistry, University of Coimbra, Coimbra, Portugal P-3049, (351) 39-852080, Fax (351) 39-827703, e-mail: rfausto@gemini.ci.uc.pt, http://qui.uc.pt/ ~ rfausto/eucmos_xxv

♦ AUGUST 27-SEPTEMBER 1, 2000

15th INTERNATIONAL MASS SPECTROMETRY CONFERENCE
Barcelona, Spain.

Information: Ana Costeja, Palau de Congressos, Departament de Convencions, Av. Reina Mª Cristina, s/n, 08004 Barcelona, Spain (34) 932-332-377, Fax (34) 934-262-845, e-mail: 15imsc@website.es, http://www.website.es/15imsc

SEPTEMBER 3-7, 2000

16th INTERNATIONAL CONFERENCE ON HIGH RESOLUTION MOLECULAR SPECTROSCOPY
Prague, Czech Republic.

Information: S. Urban, UFCH JH Academy of Sciences of the Czech Republic, Dolejskova 3, Prague, Czech Republic, CZ-18223, (420) 2-6605-3635, Fax (420) 2-858-2307, e-mail: praha2k@jh-inst.cas.cz, http://www.chem.uni-wuppertal.de/conference/

SEPTEMBER 10-13, 2000

3rd EUROPEAN THERMAL SCIENCES CONFERENCE
Heidelberg, Germany.

Information: E. Hahne, Institut fur Thermodynamik und Warmetechnik, Pfaffenwaldring 6, 70550 Stuttgart, Germany, 49 (0) 711-685-3536, Fax 49 (0) 711-685-3503, e-mail: pm@itw.uni-stuttgart.de

SEPTEMBER 10-15, 2000

CONFERENCE ON LASERS AND ELECTRO-OPTICS (CLEO) AND THE INTERNATIONAL QUANTUM ELECTRONICS CONFERENCE (IQEC)
Nice, France.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org

♦ SEPTEMBER 10-15, 2000

1st INTERNATIONAL SYMPOSIUM ON MICROGRAVITY RESEARCH AND APPLICATION IN PHYSICAL SCIENCES AND BIOTECHNOLOGY
Sorrento, Italy.

Information: ESTEC, Conference Bureau, P.O. Box 299, 2200 AG Noordwijk, The Netherlands, (71) 5655005, Fax (71) 5655658, e-mail: confburo@estec.esa.nl

♦ SEPTEMBER 12-14, 2000

3rd UNITED KINGDOM MEETING ON COAL RESEARCH AND ITS APPLICATIONS
Birmingham, UK.

Information: H.J. Graham, Power Technology Centre, Radcliffe-on-Soar, Nottingham NG11 0EE, UK, 44(0)115-936-2460, Fax 44(0)115-936-2205, e-mail: helen.graham@powertech.co.uk

SEPTEMBER 13-16, 2000

2nd INTERNATIONAL CONFERENCE ON INORGANIC MATERIALS
Santa Barbara CA.

Information: Sarah Wilkinson, Conference Secretariat, Elsevier Science Ltd., The Boulevard, Langford Lane, Kidlington, Oxford, UK OX5 1GB, 44(0) 1865 843691, Fax 44(0) 1865 843658, e-mail: sm.wilkinson@elsevier.co.uk, http://www.elsevier.com/locate/im2000

SEPTEMBER 18-20, 2000

13th INTERNATIONAL SYMPOSIUM ON GAS FLOW AND CHEMICAL LASERS AND HIGH POWER LASER CONFERENCE
Florence, Italy.

Information: C. Pescucci, Fax 39(0) 55-233-7755, e-mail: gcl-hpl@ino.it, www.ino.it/GCL-HPL or www.es.titech.ac.jp/~kkasuya/gcl-web/index.html

SEPTEMBER 19-21, 2000

THE HYDROGEN ENERGY FORUM 2000
Munich, Germany.

Information: The Future Energies Forum, "Forum fur Zukunftsenergien", Godesberger Allee 90, D-53175 Bonn, Germany, Fax 49(0) 228-959 56-50, e-mail: energie.forum@t-online.de

SEPTEMBER 22-30, 2000

27th Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies
Nashville TN.

Information: Division of Analytical Chemistry, FACSS, (505) 820-1648, Fax (505) 989-1073, Web Site: http://FACSS.org/info.html

SEPTEMBER 23-26, 2000

ASME Fall Technical Conference of the Internal Combustion Engine Division
Peoria IL.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

SEPTEMBER 24-26, 2000

1st Romanian International Conference on Analytical Chemistry
Brasov, Romania.

Information: G.L. Radu, University of Bucharest, Faculty of Chemistry, 4-12, Elisabeta Blvd., Bucharest, Romania 703461, 40(1) 220 77 80/220 79 09, Fax 40(1) 220 76 95, e-mail: lucian@ibd.dbio.ro

♦ SEPTEMBER 29-30, 2000

Four Corners Section Fall Meeting of the American Physical Society
Fort Collins CO.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 2-5, 2000

ICALEO 2000, International Conference on Applied Laser Applications and Electrooptics
Dearborn MI.

Information: E. Cohen, Laser Institute of America, (800) 345-2737 or (407) 380-1553, Fax (407) 380-5588, http://www.laserinstitute.org

OCTOBER 8-11, 2000

Gasification Technologies Conference
San Francisco CA.

Information: M. Samoulides, (650) 855-2127, or Electric Power Research Institute, 1412 Hillview Avenue, Palo Alto, CA 94304, (650) 855-2599, http://www.epri.com

♦ OCTOBER 13-14, 2000

OHIO SECTION FALL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Toledo, OH.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 16-19, 2000

INTERNATIONAL FUEL AND LUBRICANTS FALL MEETING AND EXPOSITION OF THE SOCIETY OF AUTOMOTIVE ENGINEERS
Baltimore MD.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, Web Site: http://www.sae.org

♦ OCTOBER 19-20, 2000

SAMPLING, ON-SITE ANALYSIS AND SAMPLE PREPARATION CONFERENCE
Pittsburgh PA.

Information: B. Sherman, PACS, 409 Meade Dr., Coraopolis, PA 15108, (724) 457-6576 or (800) 367-2587, Fax (724) 457-1214, e-mail: hnpacs@aol.com, http://members.aol.com/hnpacs/pacs.htm

OCTOBER 22-27, 2000

198th NATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY
Phoenix AZ.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/198/meet.html

OCTOBER 24-27, 2000

53rd ANNUAL GASEOUS ELECTRONICS CONFERENCE OF THE AMERICAN PHYSICAL SOCIETY
Houston TX.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 25-28, 2000

35th MIDWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
St Louis MO.

Information: C.D. Spilling, Department of Chemistry, University of Missouri, St. Louis, 80001 Natural Bridge Road, St. Louis, MO 63121 (314) 516-5313, Fax (314) 553-5342, e-mail: cspill@umsl.edu

♦ OCTOBER 25-28, 2000

36th Western Regional Meeting of the American Chemical Society
San Francisco CA.

Information: N.D. Byington, Customs Service Laboratory, 630 Sansome Street, Room 1429, San Francisco, CA 94111, (415) 705-4405 ext. 216, Fax (415) 705-4236, e-mail: byington@crl.com; or S. Rodriguez, Chemistry Department, University of the Pacific, Stockton, CA 95211, (209) 946-2598, Fax (209) 946-2607, e-mail: srodriguez@uop.edu

♦ OCTOBER 28-29, 2000

Joint Fall Meeting of the Texas Sections of the aps, appt and Zone 13 of the sps
Houston TX.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 29-NOVEMBER 3, 2000

Eastern Analytical Symposium of the American Chemical Society
Atlantic City NJ.

Information: S. Gold, Eastern Analytical Symposium, P.O. Box 633, Montchanin, DE 19710 (302) 738-6218, Fax (302) 738-5275, http://www.eas.org

♦ NOVEMBER 1-2, 2000

Computational and Experimental Methods in Reciprocating Engines
London UK.

Information: U. Otuonye, Conference and Events Department C587, Institution of Mechanical Engineers, 1 Birdcage Walk, London SW 1H 9JJ, UK, (0) 207-304-6864, Fax (0) 207-222-9881, e-mail: u_otuonye@imeche.org.uk

NOVEMBER 2-4, 2000

Southeast Section Meeting of the American Physical Society
Starkville MS.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

NOVEMBER 3-8, 2000

Photonics East
Boston MA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

NOVEMBER 5-10, 2000

ASME INTERNATIONAL MECHANICAL ENGINEERING CONFERENCE AND EXHIBITION
Orlando FL.

Symposia will Include:

- Symposium on Multiphase Flow in Biomedical Applications and Processes
- Dispersed Flows in Combustion, Incineration, and Propulsion Systems
- Application of Microfabrication to Fluid Mechanics

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

NOVEMBER 5-10, 2000

INTERNATIONAL SYMPOSIUM ON MULTIPHASE FLOW AND TRANSPORT PHENOMENA
Antalya, Turkey.

Topics will Include:

- Modeling of Multiphase Systems
- Transport Phenomena in Multiphase Systems
- Separation Phenomena, Processes and Equipment
- Measurement and Instrumentation
- Characteristic and Effective Properties of Multiphase Systems
- Bio-Aerosols and Bio-Systems
- Surface and Interfacial Phenomena
- Pollution Control Technology
- Clean Room Technology
- Multiphase Systems Applications
- Scaling Laws for Two-Phase Flow Phenomena
- Scaling Laws for Multiphase Flow

Information: D.M. Maron, Center for Technological Education Holon, POB 305, Holon 58102, Israel, (972) 3-502 6501, Fax (972) 3-502 6510, e-mail: barad_r@barley.cteh.ac.il, http://ichmt.me.metu.edu.tr/upcoming-meetings/MFTP-00/announce.html

NOVEMBER 5-10, 2000

UNITED ENGINEERING FOUNDATION CONFERENCE ON LEAN COMBUSTION TECHNOLOGY AND CONTROL
Santa Fe NM.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, e-mail: engfnd@aol.com http://www.engfnd.org/engfnd/conf.html, or from D. Dunn-Rankin, University of California at Irvine, CA, or R.K. Cheng, Lawrence Berkeley National Laboratory.

NOVEMBER 12-17, 2000

ANNUAL MEETING OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS
Los Angeles, CA.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 3 Park Avenue, New York, NY 10016, (212) 591-7325, Fax (212) 591-8894, e-mail: meetmail@aiche.org, http://www.aiche.org

NOVEMBER 13-18, 2000

EASTERN ANALYTICAL SYMPOSIUM OF THE AMERICAN CHEMICAL SOCIETY
Somerset NJ.

Information: S. Gold, Eastern Analytical Symposium, P.O. Box 633, Montchanin, DE 19710, (302) 738-6218, Fax (302) 738-5275, Web Site: http://www.eas.org

NOVEMBER 19-21, 2000

DIVISION OF FLUID DYNAMICS MEETING OF THE AMERICAN PHYSICAL SOCIETY
Washington DC.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

NOVEMBER 27-DECEMBER 1, 2000

FALL MEETING OF THE MATERIALS RESEARCH SOCIETY
Boston MA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, http://www.mrs.org

♦ DECEMBER 3-9, 2000

6th RIO SYMPOSIUM ON ATOMIC SPECTROMETRY
Concepcion and Pucon, Chile.

Information: C.G. Bruhn, Departamento de Analisis Instrumental, Facultad de Farmacia, Universidad de Concepcion, P.O. Box 237, Concepcion, Chile, (56) 41-204252, Fax (56) 41-231903, e-mail: cbruhn@udec.cl, http://www.udec.cl/6riosymp/

DECEMBER 6-8, 2000

JOINT 52nd SOUTHEAST/56th SOUTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
New Orleans LA.

Information: A. Pepperman, SRRC, USDA-ARS, 1100 Robert E. Lee Boulevard, New Orleans, LA 70179, (208) 286-4510, Fax (208) 286-4367, e-mail: abpep@nola.srrc.usda.gov

DECEMBER 14-19, 2000

INTERNATIONAL CHEMICAL CONGRESS OF PACIFIC BASIN SOCIETIES
Honolulu HI.

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

MARCH 4-8, 2001

THE PITTSBURGH CONFERENCE, PITTCON 2001
New Orleans LA.

Information: The Pittsburgh Conference, 300 Penn Center Boulevard, Suite 332, Pittsburgh, PA 15235, (412) 825-3220, Fax (412) 825-3224, e-mail: pittconinfo@pittcon.org, http://www.pittcon.org/

MARCH 12-16, 2001

ANNUAL MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY
Seattle WA.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MARCH 25-30, 2001

199th NATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY
Washington DC.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/199/meet.html

APRIL 1-5, 2001

221st NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Diego CA.

Division of Fuel Chemistry:
- CO_2 Capture and/or Utilization Reaction Mechanisms in Fuel Processing
  P.F Britt, Chemistry Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831, (423) 574-5029, Fax (423) 576-5235, e-mail: brittpf@ornl.gov
- Coal Bed Methane
  P.C. Thakur, Consol Inc., R&D, 1027 Little Indian Creek Road, Morgantown, WV 26501, (304) 983-3207, Fax (304) 983-3209, e-mail: promodthakur@consolcoal.com
- Nitrogen Chemistry in Coal Utilization
  M.A. Wojtowicz, Advanced Fuel Research Inc., 87 Church Street, East Hartford, CT 06108, (860) 528-9806 ext 142, Fax (860) 528-0648, e-mail: marek@afrinc.com
- Hydrogen Energy
  R. Khan, Texaco Inc., P.O. Box 509, Beacon, NY 12508, (914) 838-7639, Fax (914) 838-7102
- Argonne National Lab Premium Coal Sample Database

K. Vorres, 27 Windward Circle, Willowbrook, IL 60514, (630) 325-0931 [between Nov. 11 and April 15: 3432 North Applewood, Tucson, AZ 85712-5478, (520) 322-5256], e-mail: ksvorres@flash.net

- Carbon Products for Environmental Applications
  A. Lizzio, Illinois State Geological Survey, 615 East Peabody Drive, Champaign, IL 61801, (217) 244-4985, Fax (217) 333-8566, e-mail: lizzio@geoserv.isgs.uiuc.edu

APRIL 16-20, 2001

SPRING MEETING OF THE MATERIALS RESEARCH SOCIETY
San Francisco CA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, http://www.mrs.org

APRIL 23-27, 2001

APRIL NATIONAL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Washington DC.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MAY 6-11, 2001

CLEO/QELS 2001
Baltimore MD.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org, http://www.osa.org/mtg_conf

MAY 20-25, 2001

FLUIDIZATION X
Beijing, China.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, http://www.engfnd.org/engfnd/conf.html

MAY 20-25, 2001

2nd INTERNATIONAL SYMPOSIUM ON ADVANCES IN COMPUTATIONAL HEAT TRANSFER
Cairns, Australia.

Information: F. Arinc, Secretary-General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210-1429, Fax (90) 312-210-1331, arinc@metu.edu.tr, http://ichmt.me.metu.edu.tr

MAY 30-JUNE 1, 2001

35th Middle Atlantic Regional Meeting of the American Chemical Society
Baltimore MD.

Information: L.J. Boucher, Towson University, Department of Chemistry, 8000 York Road, Towson, MD 21252-0001, (410) 830-3057, Fax (410) 830-4265, e-mail: lboucher@towson.edu

♦ JUNE 11-13, 2001

Joint Central/Great Lakes Regional Meeting of the American Chemical Society
Grand Rapids MI.

Information: R.J. McCabe, Parke-Davis Pharmaceuticals, 188 Howard Ave., Holland, MI 49424, (616) 392-2375 ext. 2386, Fax (616) 392-8916, e-mail: Richard.McCabe@wl.com

JUNE 13-15, 2001

Joint 33rd Central/33rd Great Lakes Regional Meeting of the American Chemical Society
Grand Rapids MI.

Information: R.J. McCabe, Parke-Davis, 188 Howard Avenue, Holland, MI 49423, (616) 392-2375 ext 2386, Fax (616) 392-8916, e-mail: Richard.McCabe@wl.com

JUNE 13-16, 2001

56th Northwest Regional Meeting of the American Chemical Society
Seattle WA.

Information: S. Jackels, Department of Chemistry, Seattle University, 900 Broadway, Seattle, WA 98122, (206) 296-5946, Fax (206) 296-5786, e-mail: sjackels@seattleu.edu

♦ JUNE 24-27, 2001

30th Northeast Regional Meeting of the American Chemical Society
Durham NH.

Information: H. Mayne, Chemistry Department, University of New Hampshire, Durham, NH 03824, (603) 862-1550, e-mail: howard.mayne@unh.edu

JUNE 24-28, 2001

Annual Meeting of the Air and Waste Management Association
Orlando FL.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org

♦ JULY 1-6, 2001

GORDON RESEARCH CONFERENCE ON LASER DIAGNOSTICS IN COMBUSTION
Mount Holyoke College, South Hadley MA.

Information: J.B. Jeffries, Molecular Physics Laboratory, SRI International, 333 Ravenswood Ave., Menlo Park, CA 94025, (650) 859-6341, Fax (650) 859-6196, e-mail: jay.jeffries@sri.com

JULY 9-11, 2001

COMBUSTION CHEMISTRY: ELEMENTARY REACTIONS TO MACROSCOPIC PROCESSES: FARADAY DISCUSSION NUMBER 119
Leeds, UK.

Joint Meeting with the British Section of the Combustion Institute.
Information: M. Pilling, School of Chemistry, University of Leeds, Leeds UK, e-mail: m.j.pilling@chem.leeds.ac.uk, http://www.chem.leeds.ac.uk

AUGUST 20-24, 2001

13th INTERNATIONAL CONFERENCE ON FOURIER TRANSFORM SPECTROSCOPY
Turku, Finland.

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AUGUST 26-30, 2001

222nd NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Chicago IL.

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

SEPTEMBER 2-7, 2001

200th NATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY AND THE 52nd MEETING OF THE INTERNATIONAL SOCIETY OF ELECTROCHEMISTRY
San Francisco CA.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/198/meet.html

SEPTEMBER 23-27, 2001

52nd SOUTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Savannah GA.

Information: G. Novotnak, Kemira Pigments, 104 Carlton Road, Savannah, GA 31410, (912) 652-1290, Fax (912) 897-1163, e-mail: george.novotnak@kemira.com

SEPTEMBER 23-27, 2001

6th World Congress of Chemical Engineering: A New Century of Chemical Engineering
Melbourne, Australia.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 3 Park Avenue, New York, NY 10016, (212) 591-7325 or (800) 242-4363, Fax (212) 591-8894, e-mail: meetmail@aiche.org, http://www.aiche.org

OCTOBER 5-12, 2001

28th Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies
Detroit MI.

Information: C. Lilly, Federation of Analytical Chemistry and Spectroscopy Societies, 1201 Don Diego Ave., Santa Fe, NM 87505, (505) 820-1648, Fax (505) 989-1073, e-mail: jsjoberg@trail.com, http://facss.org/info.html

OCTOBER 10-13, 2001

36th Midwest Regional Meeting of the American Chemical Society
Lincoln NE.

Information: D. Berkowitz, Department of Chemistry, University of Nebraska, Lincoln, NE 68588-0304, (402) 472-2738, Fax (402) 472-9402, e-mail: dbb@unlinfo.edu

OCTOBER 14-19, 2001

International Symposium on Visualization and Imaging in Transport
Antalya, Turkey.

Information: F. Arinc, Secretary-General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210-1429, Fax (90) 312-210-1331, arinc@metu.edu.tr, http://ichmt.me.metu.edu.tr

OCTOBER 16-19, 2001

57th Southwest Regional Meeting of the American Chemical Society
San Antonio TX.

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OCTOBER 23-26, 2001

36th WESTERN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Ventura CA.

Information: R.W. Hurst, 9 Faculty Court, Thousand Oaks, CA 91360, (805) 492-7764, Fax (805) 241-7149, e-mail: Alarwh@aol.com

NOVEMBER 26-30, 2001

FALL MEETING OF THE MATERIALS RESEARCH SOCIETY
Boston MA.

Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, e-mail: info@mrs.org

CURRENT BIBLIOGRAPHY RELEVANT TO
FUNDAMENTAL COMBUSTION
September 1999

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Vortex Ring
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Flame Propagation
Flow Visualization
C_3H_8/Air

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Laminar
Couette Flow
Lower Wall
Fuel Injection
Upper Wall
Withdrawal
Theory

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Buoyant
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Modeling

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Counterflow
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Theory

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Lifted Jet
Diffusion Flame
Leading Edge
Stabilization
CH,PLIF
Measurements

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Diffusion Flame
CH_4/Air
$(CH_3)_2CO$,LIF
Mixing
Flow Maker

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Diffusion Flames
H_2 Gas Jet
Microgravity
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Oscillatory
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Flow Structure
Schlieren

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Crossflow Flames
Combustion
Efficiencies
Measurement
Method

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Combustion
Enhancement
Discharged
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Injection
Gas Turbine

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C_2H_2/O_2
C_2H_5OH/O_2
Flame Front
CH, C_2, OH
Spectral Emissions

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Propagation
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Fuel/Air
Ratio Monitor
Ion Current
Diagnostic
$(CH_3)_2CO$ Dopant
2-D LIF
Comparisons

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Slit,Tube
Burners
Laminar CH_4/Air
Critical Gradients

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Closed Tube
Combustion
Propagation
Acoustic Wave
Effects
Modeling

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Instabilities
Thermoacoustic
Gas Turbine
OH Emission
Visualization
Active Control
Method
NO Effects

12. TURBULENCE

(See also Section 14 for Turbulent Flame Velocities and Flowfields)

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Turbulent
Flames
Fractal Dimension
Theory

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Turbulent
Combustion Theory
Perturbed Flames
Lewis Number
Effects

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Turbulent
Combustion
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Wavelet Based
Method

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Reacting Flows
Low Mach Number
Adaptive Mesh
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CFD,Reduced
Kinetics

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Turbulent
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Practical CFD
Modeling
4 Kinetic
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Adequacies

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Turbulent
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Mixing Model
Testing

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Turbulent
Counterflow
Premixed Flames
Coherent
Flamelet Model

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Turbulent
Premixed Flames
Stagnation Flow
Stabilization
Modeling

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Turbulent
Premixed Flames
Surface
Orientation
Laser Tomography
Measurements

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Turbulent
Premixed Flames
CO/H_2/Air
Kinetic
Approximation
Method

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Turbulent
Supersonic Flows
Multigrid
Modeling Method

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Supersonic
Reacting Flows
Kinetics,CFD
CH_4,H_2/Air
Multigrid Method

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Turbulence
Combustion
Generated
Partially Premixed
Supersonic
Diffusion Flame
Heat Release
Modeling

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Turbulent
Reactive Flows
PDF Solver
Method

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Turbulence
PDF Modeling
Scalar Mixing
Reacting Layer

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Reacting Flows
Composition PDF
Transport
Modeling

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Turbulent
Diffusion Flames
1-D Raman
PDF Determination

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Turbulent
Piloted CH_4/Air
Diffusion Flame
PDF
Calculations

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Turbulent
H_2/Air
Jet Diffusion
2nd Order
Closure Term

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Turbulent Flames

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Turbulent
H_2/Air
Diffusion Flame
Flamelet Model
NO Predictions

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Turbulent
Lifted CH_4/Air
Jet Flame
Coflow Velocity
Liftoff Effects
Modeling

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Turbulent
CH_4 Jet Flame
Heated Coflowing Air
Lift-off/NO
Reduced Emissions

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Turbulent
Lifted
CH_4 Piloted
Jet Flame
Air Crossflow
CH*,OH PLIF
Stabilization
Structure

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Turbulent
Lifted Diffusion
H_2 Flames
Stabilization
Point
Raman/Rayleigh
PLIF,OH

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Turbulent
H_2 Jet Flames
Liftoff Heights
Flame Lengths

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Turbulent
Jet Flames
PLIF,OH
PIV Velocities
Vorticity/
Strain
Relationship

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Turbulent
Piloted CH_4/Air
Jet Flames
Rayleigh
Raman,LIF
Species PDFs

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Turbulent
C_2H_4/Air Jet
Soot,LII
PAH,LIF
Measurements

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Turbulent
C_3H_8/Air
Multijet Flames
Interaction
Effects
LDV
Measurements

(82576) Gas/Liquid Droplet, Mixing/Reaction Model | Turbulent Shear Flow

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Turbulent
H_2/Liquid O_2
Predissociative
O_2,LIF
2-D Imaging

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Turbulent
Diffusion Flame
Air Crossflow
Soot Effects
Modeling

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Turbulent
Bluff Body
Stabilized Flame
Recirculation
Flow Structure
Rayleigh
Raman,LIF

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Turbulent
Diffusion Flame
Bluff Body
Stabilized Structure

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Turbulent
Bluff Body
Lean CH_4/Air
PDF Model
Reduced Kinetics
Accuracies

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Turbulent
Bluff Body
Stabilized
CH_4,C_3H_8
Diffusion Flames
Extinction
Modeling

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Turbulent
Bluff Body
Stabilized
CH_4/H_2/Air
Reduced Kinetics
Model

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Turbulent
Swirling Flows
Prevaporized
Fuel Oil
Combustor
Design Requirements
NO_x Emissions

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Turbulent
Swirling Flame
Flow Structure
Natural Gas
2 Component LDV
Rayleigh
LIF,OH

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Turbulent
Nonpremixed
CH_4 ,N_2 Raman
Piloted Flames
Mixture Fraction
Imaging

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Turbulent
CH_4/Air
ps LIF,CH,OH
Minor Species
Fluctuations
Mixture Fractions

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Turbulent
Reacting
Duct Flows
Porous Wall
CH_4 Injection
Numerical Model

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Turbulent
Diluted H_2 Flame
Stability
Rayleigh/Raman
LIF,OH,LDV
PDF Model

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Detonation
Shock Dynamics
Asymptotic
Theory

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C_2H_2/Air
Turbulent
Flame Brush
Hot Spot Role
Numerical Model

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Cell Size

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C_3H_8, H_2
Propagation
Energy Release

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Modeling

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Starch Particles
H_2/O_2 Mixtures
Propagation
Heat Release
Modeling

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Flowfield
Modeling

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Heat Release

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Vortex Wake Structure
Aircraft Flowfield
Model

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(82629)	C_3H_8/Air Vortex Ring, Laser Ignition, Flame Propagation	Flow Visualization
(82827)	Incineration Performance	Fluid Flow Modeling
(82636)	Oscillatory H_2 Jet Diffusion Flame, Schlieren	Flow Structure
(82634)	CH_4/Air Diffusion Flame, $(CH_3)_2CO$ LIF	Mixing Flow Marker
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(82879)	Particles, Sizes, Velocities, Methods	LDA,PDA
(82623)	CH_4/Air Triple Flames, Structure, Temperatures, Kinetic Modeling	LDV
82723.	Davis, S.G., and C.K. Law, "Determination of and Fuel Structure Effects on Laminar Flame Speeds of C_1 to C_8 Hydrocarbons," *Combust. Sci. Technol.* 140, 427-449 (1998).	Flame Speeds C_1-C_8 Hydrocarbons Alcohols Counterflows Structure Effects Measurements
(83055)	C_3H_6 Pyrolysis, C_3H_6/O_2, Flow Reactor, Species Profiles, Kinetic Modeling Uncertainties	Flame Speeds
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Forcing Effects
Theory

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Stretch Effects
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Model

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Premixed
Burning Velocities
Lifted Jet Flames
Large Eddy
Propagation
Modeling

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Diffusivities
10 Species
Air,N_2,O_2
Review

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Transport
Parameters
SiF_4,$SiCl_4$
Diffusion
Viscosities
200-840 K

15. IONIZATION

(See also Section 26 for Ion Spectroscopy, Section 40 for Dynamics of Ion-Molecule Reactions, Section 42 for REMPI, Section 43 for Ion P.E. Curves and Surfaces, Section 44 for Ionic Structures and Section 46 for Thermochemical Values)

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Anions
Atoms,Molecules
Gas Phase
Stabilities
Review

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Anion Emissions

(83024) Hydrocarbon Monitor, Vehicle Emissions, IR Absorption Comparisons
FID

(83025) Atmospheric Hydrocarbons Monitor, O_3 Chemiluminescent Monitor Comparisons, Sensitivities, 27 Organics
FID

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(83171) Unimolecular Dissociation, Channels, Measurements $C_2H_3F^+$ $C_2H_2F_2^+$

(82884) Photoionization Cross Sections, Seven Valence States, Calculations C_{60}

(82931) Dissociative Electron Attachment Spectrum, Analysis ClO_2

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(83017) Transition Probabilities, Lifetimes, Calculations Co^+, Fe^+

(83044) LIF Measurements, Densities Monitor, Rayleigh Scattering Calibration Fe^+, Fe

(82939) Ionization Limits, GeO Vacuum Ultraviolet Absorption Spectrum $GeO^+(C,B,A,X)$

(83137) Dissociation Cross Sections, H, Cl Products, Calculations $HCl + e^-$

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(83143)	Probabilities, Numerical Modeling	IR MPD H_2^+,HD^+,D_2^+
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(83147)	fs Photoionization, Protonated Product Cluster Ions, Unimolecular Dissociation	$(H_2O)_n + h\nu$ $(D_2O)_n + h\nu$
(82997)	Penning Ionization, CO_2^+(C,B,A,X) Product Ions, Cross Sections	$He(2^1S) + CO_2$
(82998)	Penning Ionization, Cross Sections	$He(2^3S) + C_2N_2$
(82999)	Penning Ionization, Cross Sections	$He(2^3S) + HCNO$ $He(2^3S) + HN_3, N_2O$
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(83150) (83151)	fs Photoelectron Spectra, I_2^-, I^- Products, Dynamics	$I_3^- + h\nu$
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(82958)	Rydberg States, Predissociation, Electric Field Effects, Analysis	NO Autoionization
(82853) (82854)	e^- Beam, Discharge Methods, Flue Gases	NO_x Control

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(83329)	Vibrational Energy Transfer, Cross Sections, Calculations	$N_2^+(v=2,1) + N_2$
82743.	Blomberg, M., S.S. Yi, R.J. Noll and J.C. Weisshaar, "Gas Phase $Ni^+(^2D_{5/2}) + n\text{-}C_4H_{10}$ Reaction Dynamics in Real Time: Experiment and Statistical Modeling Based on Density Functional Theory," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7254-7267 (1999).	$Ni^+ + C_4H_{10}$ $Ni^+ + C_4D_{10}$ Crossed Beams Products Mechanism
82744.	Scott, G.B.I., D.A. Fairley, D.B. Milligan, C.G. Freeman and M.J. McEwan, "Gas Phase Reactions of Some Positive Ions with Atomic and Molecular Oxygen and Nitric Oxide at 300 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7470-7473 (1999).	$O,O_2 + M^+$ $NO + M^+$ 7 H/C/N/O Ions Rate Constants Product Ions
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(83330)	Vibrational Relaxation, Rate Constants, P.E. Surface, Calculations	$O_2^+(v=1) + Kr$
82746.	Matejcik, S., P. Stampfli, A. Stamatovic, P. Scheier and T.D. Mark, "Electron Attachment to Oxygen Clusters Studied with High Energy Resolution," *J. Chem. Phys.* 111, 3548-3558 (1999).	$(O_2)_n + e^-$ Attachment Cross Sections Crossed Beam Measurements
(82856)	Discharge Method, Flue Gases, Heterogeneous Role	SO_2 Control

16. INHIBITION/ADDITIVES

(82555)	Diesel Fuel Additives, Ignition Delays, Cetane Number, Polar Molecule Roles	Surfactant Agents
(82847)	NO_x Control Reburn Method, Mechanisms, Kinetic Modeling	C_2H_4 Additive
(82835)	Incineration, PCCD/Fs Emissions, $(CH_3)_2NH$, NH_3, CH_3SH, SO_2 Effects	Additive Effects
(82821)	CH_4, C_2H_2 Flames, PAH Formation, Additive Effects, Soot Role	$Fe(C_5H_5)_2$
(83196)	CH_4/CH_3OH Conversion, Reaction Dynamics, P.E. Surfaces, Crossing Seams, Energies, Calculations	FeO^+ Catalysis
(82851)	NO_x Control, Flue Gases, Oxidation/Scrubbing Method	H_2O_2 Additions
(82613)	Ignition Effects, Hydrocarbons, H_2 with Counterflowing Air, Temperatures, Kinetic Modeling	NO Additive

(82848) (82849) Natural Gas Addition, Modeling — NO_x Control, Reburn Method

(82837) PCCD/Fs Formation, Incineration, Effects — NaCl Additive

17. CORROSION/EROSION/DEPOSITION

(See also Section 22 for Diamond Formation Deposition)

18. GAS/SURFACE INTERACTIONS/BOUNDARY LAYER COMBUSTION

(See also Section 7 for Catalytic Combustion and Section 22 for Particle Formation and Deposition)

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Downward Propagation
Radiative Heat Transfer
Influence

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Thick Solid
Downward Propagation
Model

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Flame Spread
Thin/Thick Fuels
Downward Propagation
Thickness Effects

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Downward Propagation
Paper Sheets
2-D Model

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Flame Spread
Solid Fuel
Forced Flow
Velocities
Structure
Modeling

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Flame Spread
Fuel Rod
Zero Gravity
Rates
Modeling

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82754.	Kim, I., D.N. Schiller and W.A. Sirignano, "Axisymmetric Flame Spread Across Propanol Pools in Normal and Zero Gravities," *Combust. Sci. Technol.* 139, 249-275 (1998).	Flame Spread C_3H_7OH Pools Propagation Gravity Effects
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(82823)	Combustion, Toxic Metal Emission Control, Review	Sorbents
(82825)	Hg Emission Control Sorbent	Activated Carbon
(82832)	Interaction, Incineration	Fly Ash/$HgCl_2$
(82857)	Interactions, SO_3 Formation	Ash/SO_2
(82834)	PAH Emissions, Incineration, Fly Ash Content, Carbon, Metal Influences	Catalytic Formation
(82836)	PCDD/F Formation, Incineration, Cu, Metals/Fly Ash Interaction Effects	Catalytic Formation
(82846)	NO_x Control Method, Kinetic Model	Alkene/Catalyst
(82845)	NO Control Method	NH_3/Catalyst

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Heterogeneous
$HCl+HOCl$
Ice Surface
Cl_2 Product
Calculations

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Heterogeneous
HCl,HNO_3/Ice
SO_2/Ice
Uptake Effects
Evaporative
Changes

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Heterogeneous
HOBr/Ice
Uptake
Coefficient
HOBr+HCl
Probabilities

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Heterogeneous
HONO/Aerosol
NO_2/Aerosol
NaCl,$(NH_4)_2SO_4$
Rate Constants

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NO_2/H_2SO_4aq
Conversions
HONO Formation
Atmospheric
Implications

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(See also Section 10 for Ignition)

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Handbook

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I.C. Engines
1-, 2-Zone
Turbulence Model
Evaluations
Adequacies

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Vehicle Emissions

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Alternate Fuels
Evaporative Losses
Emission
Components
Testing

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Auto Emissions
VOCS
Particle Bound
Organics
221 Compounds
Measurements

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Auto Emissions
C_2-C_{10} Hydrocarbons
South American
Fuel Effects

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I.C. Engines
C_3H_8 Fueled
Exhaust Port
UHC Sampling

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I.C. Engines
Particulate
Emissions
Size
Distributions

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I.C. Engines
Emissions Control
Catalytic
Converter
Dominant
Importance

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Diesel Engine
Liquid Fuel
Penetration
Model/
Measurement
Comparisons

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82776.	Morawska, L., N.D. Bofinger, L. Kocis and A. Nwankwoala, "Submicrometer and Supermicrometer Particles from Diesel Vehicle Emissions," *Environ. Sci. Technol.* 32, 2033-2042 (1998).	Diesel Engine Particulates Sizing Measurements
82777.	Reitz, R.D., "Controlling Direct Injection Diesel Engine Emissions Using Multiple Injections and Exhaust Gas Recirculation," *Combust. Sci. Technol.* 138, 257-278 (1998).	Diesel Engine Emissions Control High Pressure Fuel Injection EGR Soot,NO Reductions

20. PLUME/STACK CHEMISTRY/ATMOSPHERIC EMISSIONS

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C_2F_4

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7 Fluoroethers

(83095) OH Reaction Rate Constants, Atmospheric Lifetimes

13 Ethers

(83098) Atmospheric Lifetimes, OH Reaction Rate Constants

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Measurements

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Soot Condensation
Modeling

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Combustion
Energy Recovery
Optimal
Moisture Content

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Low CO,NO
Emissions

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Emissions

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Reburn Method
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NO Control
Measurements

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Mechanisms
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PAHS
Emissions
Testing

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PAH Emission
Fly Ash Content
Carbon,Metal
Effects

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Incineration
PCDD/Fs
Emissions
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CH_3SH,SO_2
Additive Effects

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PCDD/F
Formation
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Catalysis

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Incineration
PCDD/Fs
Emissions
NaCl Addition
Effects

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Kinetic Modeling
$CH_4/O_2/N_2$
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Model Testing
Accuracies

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Heat Release
Turbulent
CH_4/Air
Reduced Kinetics
New Methodology

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C_2H_4 Addition
Reburn Method
Kinetic Modeling
Mechanisms

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Reburn Method
Mixing
Modeling

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Reburn Method
Natural Gas
Jet Stirred
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Kinetic Modeling
Controlling Channels

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NO Control
Reburn Method
Tire Derived
Injection Fuel
Potential

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NO_x Control
Flue Gases
H_2O_2 Addition
Oxidation/
Scrubbing Method

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NO_x Control
e^- Beam Method
Removal
Efficiency

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Flue Gases
Corona Discharge
Method
Kinetic Modeling

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NO,SO_2,CO
Emission Control
Flue Gases
Corona Discharge
Method

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SO_2 Control
Flue Gases
Discharge Method
Heterogeneous
Role

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SO_2/Ash
Interactions
SO_3 Formation

22. SOOT, DIAMOND, PARTICLE FORMATION/CONTROL

(See also Section 19 for Engine Soot Formation)

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Soot,PAHs
Fullerenes
Flame Formation
Overview

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Soot Inception
Counterflow
Nonpremixed Flames
Asymptotic
Analysis Model

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Soot Formation
CH_4/Air
Diffusion Flame
Reduced Kinetics
Modeling

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Soot Formation
C_2H_2/Air
Turbulent Jet
Modeling
Data Comparison

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Soot Formation
C_2H_2/Air
Diffusion Flame
Electric Field
Controlling Effects

82863. Konsur, B., C.M. Megaridis and D.W. Griffin, "Soot Aerosol Properties in Laminar Soot-Emitting Microgravity Nonpremixed Flames," *Combust. Flame* 118, 509-520 (1999).

Soot Formation
C_2H_2/Air
Jet Flame
Zero Gravity
Volume Fractions
Properties

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(83062) C_3O_2/Ar Pyrolysis, Yields, Sizes, Shock Tube	Soot Formation
82867. Fischer, B.A., and J.B. Moss, "The Influence of Pressure on Soot Production and Radiation in Turbulent Kerosene Spray Flames," *Combust. Sci. Technol.* 138, 43-61 (1998).	Soot Formation Turbulent Kerosene Spray Flames Pressure Effects
(82755) JP8 Fuel Pool Fires, Volume Fractions, Radiative Flux, Temperature Measurements	Soot Formation
(82595) Polymer Particle Combustion, Single/Group Measurements	Soot,PAH Formation
(82569) Catalytic Oxidation, Removal Methods	Diesel Soot/NO_2
(82821) Heterogeneous Surface Formation of PAHs, CH_4, C_2H_2 Flames	Soot Role
(82814) Particle Formation, Aircraft Emissions, H_2SO_4/H_2O Condensation on Soot, Modeling	Soot Role
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Diamond Formation
C_2H_2/O_2
2-D LIF
CN, C_2, H
Species Profiles

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Diamond Formation
C_2H_2/O_2
C_2, H Densities
LIF
Measurements

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Diamond Formation
$C_2H_2/H_2/O_2$
H Atom Densities
3-Photon LIF
Measurements

82873. Yoshimoto, M., K. Yoshida, H. Maruta, Y. Hishitani, H. Koinuma, S. Nishio, M. Kakihana and T. Tachibana, "Epitaxial Diamond Growth on Sapphire in an Oxidizing Environment," *Nature* 399, 340-342 (1999).

Diamond Formation
Laser Ablated
Graphite
O_2 Environment
Epitaxial
Pure Growth

82874. Matsumoto, S., Y. Asakura and K. Hirakuri, "Diamond Synthesis by Using Very High Frequency Plasmas in Parallel Plate Electrodes Configuration," *Appl. Phys. Lett.* 71, 2707-2709 (1997).

Diamond Formation
CH_4/H_2
100 MHz Discharge
Quality

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Diamond Formation
CH_4/H_2
Microwave Discharge
H Densities
Emission Monitor
$H(n=3)+H_2$
Quenching
Cross Sections

82876. Ikeda, M., H. Ito, M. Hiramatsu, M. Hori and T. Goto, "Effects of H, OH and CH_3 Radicals on Diamond Film Formation in Parallel-Plate Radiofrequency Plasma Reactor," *J. Appl. Phys.* 82, 4055-4061 (1997).

Diamond Formation
CH_4, CH_3OH
RF Discharges
H,OH Injection
Effects
Growth Rates

82877. Chis, I., A. Marcu, D. Miu, T. Yukawa, D. Dragulinescu, C. Grigoriu, W. Jiang and K. Yatsui, "Discharge Aided Reactive Laser Ablation for Ultrafine Powder Production," in *ROMOPTO '97: Fifth Conference on Optics*, V.I. Vlad and D.C. Dumitras, eds., 184 Papers Presented at a Conference Held in Bucharest, Romania, September 1997, 1228 pp., Published in 2 Volumes, Volume 1, pp. 1-639, *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3405, 188-198 (1998).

Al_2O_3
Particle Formation
$Al(s)/O_2$
Laser Ablation

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Ge
Particle Formation
Growth
GeH_4 Discharge

23. PARTICLE CHARACTERIZATION

(See also Section 5 for Spray Characterization)

(83033) In Situ Absorption, Optoacoustic, Interferometric Detection Schemes — Aerosols

(82770) Distributions, I.C. Engine Emissions — Particulate Sizes

(82776) Diesel Engine, Emissions, Measurements — Particulate Sizes

(82774) Diesel Engines, Emissions, PAH Content — Particulate Sizes

82879. Achimastos, T., M. Founti and T. Panidis, "Recent Developments in Nonintrusive Measuring Techniques for Particle Velocity and Size Measurements," in *Second Greek/Italian International Conference on New Laser Technologies and Applications*, A. Carabelas, P. Di Lazzaro, A. Torre and G. Baldacchini, eds., Proceedings of a Conference Held in Olympia, Greece, June 1997, 86 Papers, 466 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3423, 281-285 (1998).

Particles
LDA,PDA
Sizes,Velocities
Methods

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Smoke Agglomerates
Extinction
Coefficients
Polarization
Ratios
Calculations

82881. Niedziela, R.F., M.L. Norman, C.L. DeForest, R.E. Miller and D.R. Worsnop, "A Temperature- and Composition-Dependent Study of H_2SO_4 Aerosol Optical Constants Using Fourier Transform and Tunable Diode Laser Infrared Spectroscopy," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 8030-8040 (1999).

H_2SO_4/aq
Aerosols
FTIR
Optical Constants

(83146) 193 nm Photochemistry, Impurity Effects, Multiphoton Processes — H_2SO_4 Aerosols

24. NUCLEATION/COAGULATION/CLUSTERS

(See also Section 22 for Nucleation and Growth of Particles and Section 26 for Spectroscopy of Cluster Molecules)

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(83339)	Bond Energies, M = Ti thru Cu, n = 1-4, Measurements	$M^+(NH_3)_n$
(83254)	Fragment Ions, Mass Analysis, Mechanisms	MPD/MPI,$(CH_3I)_n$
(83267)	P.E. Surfaces, Construction Methods, Review	CO.He OH(A).Ar
82883.	Birkett, P.R., "Fullerene Chemistry," *Ann. Repts. Prog. Chem. A. Inorg. Chem.* 93, 611-636 (1997), 94, 55-84 (1998), 95, 431-451 (1999).	Fullerenes Synthesis Properties Chemistry Annual Reviews
(82822)	C_6H_6/O_2/Ar Flame Formation Mechanisms, Model/Measurements	C_n ,PAHS
82884.	Venuti, M., M. Stener, G. De Alti and P. Decleva, "Photoionization of C_{60} by Large Scale One-Center Density Functional Explicit Continuum Wavefunction," *J. Chem. Phys.* 111, 4589-4597 (1999).	C_{60} Photoionization Cross Sections 7 Valence States Calculations
(83360)	Measurement	$\Delta H_f(C_{70})$,s
(83309)	Structural Calculations, Geometries, ΔH_f , IP(ClCO)	$(ClCO)_2$,$(ClCO)_2^+$ ClCO,$ClCO^+$
(83296)	P.E. Surface Algorithm, Vibrational Frequencies, Calculations	$Cl^-(H_2O)$ $(H_2O)_2$
(83362)	Measurements	IP(Ge_n),n = 2-57 IP(Sn_n),n = 2-41
(83159)	Br/Br($^2P_{1/2}$), H, Product Energies, Branching Ratio, Cluster Effects	$(HBr)_n + h\nu$ $HBr + h\nu$
(83138)	Ultraviolet Photolysis, H, Cl, Ar Fragments, Wavepacket Treatment	$HCl.Ar + h\nu$
(82813)	Jet Engines, Anion Emissions, Measurements	HSO_4^-,NO_3^- Clustered Ions
(83147)	fs Photoionization, Protonated Product Cluster Ions, Unimolecular Dissociations	$(H_2O)_n + h\nu$ $(D_2O)_n + h\nu$

(83000)	Cluster Relaxation, IVR, Predissociation Mechanisms, Model, Data Comparisons	$I_2(B,v=21,22).Ne_n$
83313)	Structural Calculations, Geometries, Frequencies, Infrared Intensities	$(NO)_2^+$
(82746)	Attachment Cross Sections, Crossed Beam Measurements	$(O_2)_n+e^-$

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82886.	Taine, J., and A. Soufiani, "Gas Infrared Radiative Properties: From Spectroscopic Data to Approximate Models," *Adv. Heat Transfer* 33, 295-414 (1999).	IR Radiative Transfer CO_2, H_2O Practical Models Review
(82909)	CH_4/O_2 FTIR Flame Emission Spectrum, Assignments, Levels, Constants	CO_2, 3 μm
(82941)	C_3H_8/Air Flame, Far Infrared Rotational Absorption Spectrum	H_2O,ν_2
82887.	Pranszke, B., P. Kierzkowski and A. Kowalski, "Steric Effects in Chemiluminescent Reactions of Metastable Ca* and Sr* Atoms with Isomeric Propyl Halides," *Chem. Phys. Lett.* 309, 183-190 (1999).	Chemiluminescence $Mg(^3P_1)+C_3H_7X$ $Ca,Sr(^3P_1,^1D_2)+C_3H_7X$ X=Cl,Br,I MX(B,A-X) Cross Sections Branching Ratios
82888.	Murad, E., "The Shuttle Glow Phenomenon," *Ann. Rev. Phys. Chem.* 49, 73-98 (1998).	Chemiluminescence NO+O NO_2* Shuttle Glow

26. SPECTRAL CHARACTERIZATIONS/ANALYSES

(See also Section 43 for Energy Levels and Theoretically Calculated Spectral Constants, and Section 44 for Vibrational Frequencies and Constants)

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82892.	Andrews, D.L., *"Lasers in Chemistry,"* 3rd Edition, 5 Chapters, 232 pp., Springer-Verlag, Berlin (1997).	Laser Spectroscopy Induced Chemistry Lasers/Equipment Handbook
82893.	Kobayashi, T., "Femtosecond Phase Spectroscopy," *Ann. Repts. Prog. Chem. C. Phys. Chem.* 94, 375-395 (1998).	fs Spectroscopy Frequency Domain Interferometry Review
82894.	Sweetser, J.N., and R. Trebino, "Reduced Background Gas Phase Absorption Spectroscopy," *Opt. Lett.* 23, 1289-1291 (1998).	Absorption fs Pulsed Laser Time Gating S/N Improvement Method
82895.	Schreiber, E., *"Femtosecond Real-Time Spectroscopy of Small Molecules and Clusters,"* 6 Chapters, *Springer Tract Modern Phys.* 143, 212 pp. (1998).	fs Spectroscopy Clusters Wavepackets K_2,K_3,Na_2,Na_3 Ag_3 Overview
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82898.	Chupka, W.A., "Differential Decay of States Excited in Zero-Kinetic-Energy Spectroscopy," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 8169-8172 (1999).	ZEKE-PFI Spectroscopy Anomalous Intensities
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82902.	Larson, C.W., and J.D. Presilla-Marquez, "Vibrational Spectrum of B_2C in Argon at 10 K," *J. Chem. Phys.* 111, 1988-1992 (1999).	B_2C FTIR Spectrum Frequencies Matrix Study
82903.	Gutterres, R.F., J. Verges and C. Amiot, "The BaI($X^2\Sigma^+$) and ($B^2\Sigma^+$) Electronic States through ($B^2\Sigma^+$-$X^2\Sigma^+$) and ($C^2\Pi$-$X^2\Sigma^+$) Band Systems Analysis," *J. Mol. Spectrosc.* 196, 29-44 (1999).	BaI(B-X) Chemiluminescent LIF Spectra Analysis (C,B,X) Constants
(83344)	Photoionization Efficiency Spectra, IP(BrO,BrO_2)	BrO_2
(83345)	Ion Photoelectron Spectra, Neutral ^{1,3}Energy Splittings, Frequencies	CF_2^-,CCl_2^- CBr_2^-,CI_2^-
(83019)	(D-B) 2-Color RFWM Spectrum, D-State Constants, Predissociation Linewidths, Barrier Height	CH(D,v=0,N≤16)
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(83349)	Photoelectron Spectrum, EA, CH_3N(a,X) Energy Splitting	CH_3N^-
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Superexcited Diatomic States
CO,H_2,NO
Theory

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^{13}CO(c-a)
Emission Spectrum
Perturbations
Constants

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CO_2,3μm
FTIR Emission
CH_4/O_2 Flame
Assignments
Levels
Constants

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$CO_2^{\pm}$,$(CO_2)_2^{\pm}$
FTIR Spectra
Assignments
Frequencies
Matrix Study

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$CSCl_2(T_1\text{-}S_0)$
Absorption Spectrum
Cavity Ringdown
Assignments
T_1/S_0 Nonradiative Decay
Lifetime

82912. Sisk, W.N., N. Sarkar, S. Ikeda and H. Hayashi, "Influence of Large Magnetic Fields on Fluorescence of Gaseous CS_2 Excited Through Several V-Bands," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7179-7185 (1999).
CS_2
LIF Spectra
Several V-Bands
Magnetic Quenching

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CCH(B-X)
LIF Spectrum
Assignments
Constants
Perturbations

82914. Pochert, J., and M. Quack, "Vibrational Spectroscopy, Anharmonic Resonances, and Intramolecular Vibrational Redistribution in Tetrafluoroiodoethane," *Mol. Phys.* 95, 1055-1075 (1998).
CF_3CHFI
FTIR Spectrum
Assignments
Band Strengths
Frequencies

82915.	Heathfield, A.E., C. Anastasi, A. McCulloch and F.M. Nicolaisen, "Integrated Infrared Absorption Coefficients of Several Partially Fluorinated Ether Compounds: CF_3OCF_2H, CF_2HOCF_2H, $CH_3OCF_2CF_2H$, CH_3OCF_2CFClH, $CH_3CH_2OCF_2CF_2H$, $CF_3CH_2OCF_2CF_2H$ and $CH_2=CHCH_2OCF_2CF_2H$," *Atm. Environ.* 32, 2825-2833 (1998).	7 Fluoroethers IR Absorption Coefficients Measurements Global Warming Potential
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82917.	Herman, M., F. Herregodts, R. Georges, M. Hepp, I.H. Bachir, M. Lecoutre and I. Kleiner, "Spectroscopic Investigation of Vibration-Rotation Bands in Acetaldehyde: Focus on the $n\nu_3$(n=1-5) Aldehyde CH Stretch Bands," *Chem. Phys.* 246, 433-443 (1999).	$CH_3CHO(1\text{-}5\nu_{3(CH)})$ FT Spectrum Optoacoustic Spectral Analysis Constants
82918.	Hepp, M., and M. Herman, "Weak Combination Bands in the 3 µm Region of Ethane," *J. Mol. Spectrosc.* 197, 56-63 (1999).	C_2H_6 ,3 µm FTIR Spectrum Combination Band Analysis
82919.	Andersson, O., H. Neij, J. Bood, B. Axelsson and M. Alden, "Optical Characterization of Dimethyl Ether for Laser Based Combustion Diagnostics," *Combust. Sci. Technol.* 137, 299-322 (1998).	$(CH_3)_2O$ Laser Spectroscopy Emission,Absorption Raman,LIF CARS Characterizations
(83084)	Absorption Cross Sections	$C_3H_3Cl_2$,C_3H_3ClBr $C_3H_3Br_2$
82920.	Craig, N.C., C.F. Neese, T.N. Nguyen, C.M. Oertel, L. Pedraza and A.M. Chaka, "Vibrational Spectroscopy of the Three Isomers of 1,4-Difluorobutadiene," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6726-6739 (1999).	$C_4H_4F_2$ IR,Raman Spectra Frequencies Assignments
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82922.	Zhu, L., T. Cronin and A. Narang, "Wavelength-Dependent Photolysis of *i*-Pentanal and *t*-Pentanal from 280 to 330 nm," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7248-7253 (1999).	C_4H_9CHO Absorption Cross Sections *i*-,*t*-Structures HCO Product Yields

82923. Jalviste, E., and F. Temps, "Vibronic Spectroscopy of Jet Cooled Indazole: ($S_1 \leftrightarrow S_0$) Spectra and Mode Assignments," *J. Chem. Phys.* 111, 3898-3910 (1999).

$C_7H_6N_2(S_1-S_0)$
LIF Spectra
Assignments
Vibronic Coupling

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C_{60}
Absorption
Cross Sections
Analysis

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$C_{60}(g)$
R2PI Spectrum
High Resolution
Beam Cooling

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C_n
Fullerenes
Electronic
Absorption Spectra
Oscillator
Strengths
Calculations

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$Ca(^3D_3)Ar(^3\Sigma^+)$
R2PI Spectrum
P.E. Curve
Maximum
Constants
Perturbations

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$Ca(^3D_J).Rg(^3\Delta_{1,2})$
Rg=Ar,Kr,Xe
R2PI Spectra
Assignments
Constants

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CaCCH(A-X),ν_4
Laser Excitation
Spectrum
Analysis

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CaF(B,A)
Interactions
Spectral Analysis
Constants

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ClO_2
Absorption Spectrum
Dissociative Electron Attachment
Analysis

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ClO_2(A-X)
LIF Spectra
Unexpected Large $^{37}Cl/^{35}Cl$ Intensity Ratios

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CrO_2^-,MoO_2^-
WO_2^-,CrO_3,CrO_3^-
FTIR Spectra
Frequencies
Matrix Study

(83310) Photoelectron Spectrum, Theoretical Assignments, Structural Calculations, Frequencies

CuO_2

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FeC
LIF Spectra
Assignments
Constants
Low-lying $^5\Pi_2$ State

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$Fe(CO)_2$,ν_3
Absorption
Diode Laser
Analysis
Constants

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FeH(g-b,a,X)
FeH(e-a)
LIF Spectra
Analysis
Constants

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FeO^+(a-X)
Photofragment Spectrum
Predissociation
Lifetimes
Constants
D_0

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(83141)	^{1,3}Absorption Strengths, Contributions, Calculations	HOCl,HOBr HOI
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InI(B,A-X)
Laser Excitation
Photoionization
Spectra
B-State
Predissociation
D(InI)

82948. Ram, R.S., J. Lievin and P.F. Bernath, "Emission Spectroscopy and ab Initio Calculations on IrN," *J. Mol. Spectrosc.* 197, 133-146 (1999).

IrN(a-X)
FTIR Emission
Spectral Analysis
Constants
T_0

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K_2(X,v=36)
2-Color RPI
Monitoring
$K(^2S)+K(^2P)$
Association
(A-X) Emission
Populating

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$KrCs^+(2^1\Sigma^+-1^1\Sigma^+)$
$XeCs^+(2^1\Sigma^+-1^1\Sigma^+)$
UV Emission
Spectra
Assignments

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KrXe,ArXe
(1+1′) REMPI
Xe*(5d)
Rydberg States
Spectral Constants

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LaO,YO
LaO_2,YO_2
$LaO_2^{\pm}$,$YO_2^{\pm}$
FTIR Spectra
Frequencies
Assignments

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Li_2(B-X)
Absorption
Predissociation
Rates
P.E. Curves
B-State Barrier

82954. Chen, H., L. Li, G. Lazarov, X. Wang, A.M. Lyyra, J. Huennekens and R.W. Field, "Rotational Pattern Difference in Resolved Fluorescence Spectra with Different Detection Schemes," *J. Mol. Spectrosc.* 196, 197-211 (1999).

$Li_2(1^3\Sigma_g^- - 1(b)^3\Pi_u)$
$Li_2(1^3\Delta_g - 1(b)^3\Pi_u)$
LIF Spectra
Line Polarizations
Grating Effects
Intensities

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LnO,$LnO^\pm$
LnO_2,LnO_2^-,LnO_3^-
FTIR Spectra
Frequencies
Ln=Tb,Dy,Ho,Er
Tm,Yb,Lu
Matrix Study

(83256) MPI, Autoionizing States

Mg

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$MgCO_2$
$Mg(C_2H_4)_n$
FTIR Spectra
Frequencies
Matrix Study

(83365) Photoelectron Spectra, MoC, WC Low-lying States, Term Values, EA, Frequencies

MoC^-,WC^-

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NO,$^{15}NO(X)$
Rotational
Spectra
$^2\Pi_{1/2,3/2}$,$J\leq37.5$
Constants

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NO
Rydberg State
Autoionization
Predissociation
Electric Fields
Analysis

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$NO^+(X,v=0\text{-}32)$-NO(X)
PFI/PES Spectra
$NO^+(X)$ Constants
IP

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$NO^+(a,v=0\text{-}16)$-NO(X)
PFI/PES
Rotationally
Resolved
$NO^+(a)$ Constants
IP

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(83007) Predissociation, Spin-Orbit Coupling, Erratum — N_2^+(C)

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(83008) Spin-Orbit Coupling, Perturbations Analysis — NaK(D/d)

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82968. Yoshino, K., J.R. Esmond, W.H. Parkinson, A.P. Thorne, R.C.M. Learner and G. Cox, "Fourier Transform Spectroscopy and Cross Section Measurements of the Herzberg II Bands of O_2 at 295 K," *J. Chem. Phys.* 111, 2960-2967 (1999). — O_2(c-X); FT Absorption; Spectral Constants; Oscillator/ Line Strengths

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82970.	Song, Y., M. Evans, C.Y. Ng, C.-W. Hsu and G.K. Jarvis, "Rotationally Resolved Pulsed Field Ionization Photoelectron Bands of $O_2^+(X^2\Pi_{1/2,3/2g}$, v=0-38) in the Energy Range of 12.05-18.15 eV," *J. Chem. Phys.* 111, 1905-1916 (1999).	O_2^+(X,v=0-38)-O_2(X) Rotationally Resolved PES O_2^+(X) Constants IP
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82973.	Peterka, D.S., M. Ahmed, A.G. Suits, K.J. Wilson, A. Korkin, M. Nooijen and R.J. Bartlett, "Erratum - Unraveling the Mysteries of Metastable O_4* [*J. Chem. Phys.* 110, 6095-6098 (1999)]," *ibid.* 111, 5279 (1999).	O_2(c).O_2 Metastable Complex Photoionization PES Spectra Erratum
82974.	Ram, R.S., J. Lievin and P.F. Bernath, "Fourier Transform Emission Spectroscopy and ab Initio Calculations on OsN," *J. Chem. Phys.* 111, 3449-3456 (1999).	OsN(b,a-X) FT Emission Spectral Analysis Constants
82975.	Langenberg, J.D., L. Shao and M.D. Morse, "Resonant Two-Photon Ionization Spectroscopy of Jet Cooled PdC," *J. Chem. Phys.* 111, 4077-4086 (1999).	PdC R2PI Spectra State Assignments Constants Lifetimes
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(83110)	Deperturbation, State Couplings, Dynamics	ReN(18.5-X)
82977.	Zhou, M., and L. Andrews, "Reactions of Laser Ablated Co, Rh and Ir with CO: Infrared Spectra and Density Functional Calculations of the Metal Carbonyl Molecules, Cations and Anions in Solid Neon," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7773-7784 (1999).	RhCO,$RhCO^\pm$ FTIR Spectra Frequencies Assignments Matrix Study

82978. Li, Q., J. Shu, Q. Zhang, S. Yu, J. Dai, C. Chen and X. Ma, "Resonance-Enhanced Multiphoton Ionization Spectroscopy of SF_2 Radical," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 280-284 (1998).

SF_2
REMPI Spectra
10 Band Systems
IP

82979. Dastageer, A., E. Hegazi, A. Hamdan and F. Al-Adel, "Relative Mixing Coefficients of Zero-Order $^1B_1$(n,0,0) Levels in the ($^1B_1$-$^1A_2$) Hybrid Wave Functions of the Vibronic Bands of SO_2 in the 32184-34040 cm^{-1} Region," *J. Chem. Phys.* 111, 1784-1785 (1999).

SO_2(B-X)
LIF Spectra
B/A Mixing
Interactions
Analysis

82980. Muller, T., P.H. Vaccaro, F. Perez-Bernal and F. Iachello, "The Vibronically-Resolved Emission Spectrum of Disulfur Monoxide (S_2O): An Algebraic Calculation and Quantitative Interpretation of Franck-Condon Transition Intensities," *J. Chem. Phys.* 111, 5038-5055 (1999).

S_2O(C-X)
LIF Spectrum
Assignments
Term Values

82981. Chertihin, G.V., L. Andrews and C.W. Bauschlicher Jr, "Reactions of Laser Ablated Scandium Atoms with Nitrogen: Matrix Infrared Spectra and DFT Calculations for Scandium Nitrides and the Fixation of Nitrogen by Two Scandium Atoms," *J. Am. Chem. Soc.* 120, 3205-3212 (1998).

ScN,ScN_2
FTIR Spectra
Frequencies
Laser Ablation
Matrix Study

82982. Bredohl, H., J. Breton, I. Dubois, J.M. Esteva, D. Macau-Hercot and F. Remy, "Rydberg States of SiCl," *J. Mol. Spectrosc.* 197, 28-31 (1999).

SiCl
Rydberg States
5 New Systems
Fluorescence Spectra
$SiCl^+$(a)
Ionization Limit

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SiO(g,c-b)
Emission Spectra
Constants

82984. Focsa, C., M. Bencheikh and L.G.M. Pettersson, "The Electronic Structure of TiCl: Ligand Field versus Density Functional Calculations," *J. Phys. B. At. Mol. Opt. Phys.* 31, 2857-2869 (1998).

TiCl,$TiCl^+$
Electronic States
Energies
IP
Calculations

82985. Sakai, Y., K. Mogi and E. Miyoshi, "Theoretical Study of Low-lying Electronic States of TiCl and ZrCl," *J. Chem. Phys.* 111, 3989-3994 (1999).

TiCl
ZrCl
Low-lying
Electronic States
Energies
Spectral Constants

(83153) ($^1\Sigma^+$-$^1\Sigma^+$) Emission Spectrum, Xe/O(^{1}S) System

XeO*

82986. Simard, B., Z. Jakubek, H. Niki and W.J. Balfour, "High Resolution Molecular Beam Study of the Origin Band of the ($B^2\Sigma^+$-$X^2\Sigma^+$) System of Yttrium Imide," *J. Chem. Phys.* 111, 1483-1493 (1999).

YNH(B-X)
YND(B-X)
LIF Spectra
Geometries
Constants
Perturbations

(83371) PFI-ZEKE Spectrum, Rydberg States, D, IP(YO), YO^+ Spectral Constants

YO

82987. Adam, A.G., K. Athanassenas, D.A. Gillett, C.T. Kingston, A.J. Merer, J.R.D. Peers and S.J. Rixon, "Electronic Spectra of YOH and YOD in the Visible Region: Strong Vibronic Coupling between the $B^1\Pi$ and $C^1\Sigma^+$ States," *J. Mol. Spectrosc.* 196, 45-69 (1999).

YOH,YOD(B/C)
Vibronic Coupling
Laser Excitation
Spectra
v Levels

82988. Ram, R.S., and P.F. Bernath, "Fourier Transform Emission Spectroscopy of the $[7.3]^2\Delta$-$a^2\Phi$ and $[9.4]^2\Phi$-$a^2\Phi$ Systems of ZrCl," *J. Mol. Spectrosc.* 196, 235-247 (1999).

ZrCl($^2\Delta$,$^2\Phi$-a)
FT Emission
Spectral Constants
Assignments

82989. Brugh, D.J., R.D. Suenram and W.J. Stevens, "Fourier Transform Microwave Spectroscopy of Jet Cooled ZrO_2 Produced by Laser Vaporization," *J. Chem. Phys.* 111, 3526-3535 (1999).

ZrO_2
Rotational Spectrum
Laser Ablation
Source
Geometry
Constants

82990. Doverstal, M., L. Karlsson, B. Lindgren and U. Sassenberg, "Resonant Two-Photon Ionization Spectroscopy Studies of Jet Cooled Zr_2," *J. Phys. B. At. Mol. Opt. Phys.* 31, 795-803 (1998).

Zr_2
R2PI Spectra
3 Excited States
Assignments
Constants

27. EXCITED STATE LIFETIMES/QUENCHING

(See also Section 45 for Vibrational and Rotational Relaxation Processes)

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Fluorescence
Quenching
Excimer
Formation
Additional Channel
Theory

82992. Francis, A., U. Czarnetzki, H.F. Dobele and N. Sadeghi, "Quenching of the 750.4 nm Argon Actinometry Line by H_2 and Several Hydrocarbon Molecules," *Appl. Phys. Lett.* 71, 3796-3798 (1997).

$Ar(4p'_{1/2}) + M$
Lifetime
Quenching
Rate Constants
$M = H_2, CH_4, C_2H_2,$
C_2H_4, C_2H_6

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$Ba(^3D_1, ^{1,3}P_1) + He$
Quenching
Cross Sections
Measurements

(83268) Spin-Orbit Coupling, Predissociation Rates, P.E. Curves, D_e(B-State), Calculations

$CAr(B, 1^5\Sigma^-)$

(82911) Nonradiative Decay Lifetime, Cavity Ringdown Absorption Spectrum, Assignments

$CSCl_2(a^3A_2)$

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$CS_2(^1B_2)$
Predissociation
Lifetimes
fs Pump/Probe

(83157) CaH(v,J) Product Energy Distributions, Measurements

$Ca(^1P_1) + H_2$

(82887) X=Cl, Br, I, Metal Halide, (B,A-X) Chemiluminescence, Cross Sections, Branching Ratios

$Ca,Sr(^3P_1, ^1D_2) + C_3H_7X$
$Mg(^3P_1) + C_3H_7X$

(83275) Predissociation Lifetimes, P.E. Surface, Product States, Calculations

$Cl_2(B,v) + He$

(82937) Predissociation Lifetimes, (a-X) Photofragment Spectrum, Constants

$FeO^+(a)$

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$H(2s) + He, Ne$
Quenching
Cross Sections
Elastic Scattering
Calculations

(82875) Quenching Cross Sections, Diamond Formation Plasma Measurements

$H(n=3) + H_2$

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Quenching
Cross Sections
Room Temperature
Measurements

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Penning Ionization
$CO_2^+(C,B,A,X)$
Product Ions
Cross Sections

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$He(2^3S)+C_2N_2$
Penning Ionization
Cross Sections
$Li+C_2N_2$
Calculations

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$He(2^3S)+HCNO$
$He(2^3S)+HN_3,N_2O$
Cross Sections
Measurements
$Li+HCNO,HN_3,N_2O$
Calculations

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I_2(B,v=21,22).Ne_n
Cluster Relaxation
IVR
Predissociation
Mechanisms
Model
Data Comparisons

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Kr($^3P_1$)
Radiative
Imprisonment
Collision
Duration Effects

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Kr($4p^5nd$)
n=4-6
Lifetimes
11 Levels
Measurements

(82953) Predissociation Rates, Absorption, P.E. Curves, B-State Energy Barrier — Li_2(B,v)

(83210) Product Energies, P.E. Surfaces, Reaction Dynamics, Collision Energy Effects — $Mg(^1P_1)+H_2$

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Mo^*+CH_4
$V^*,Zr+C_2H_4$
Crossed Beams
Reactivities
Energies

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$N(^2D)+CH_3OH$
D-Isotopomers
NH,OH Products
Energy
Distributions
Mechanism

(83211) Reaction Dynamics, P.E. Surface, Energy Barriers, Channels — $N(^2D,^4S)+CH_4$

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83006.	Mo, Y., C. Ottinger and G. Shen, "Collision-Induced Intersystem Crossing from $NH(a^1\Delta,b^1\Sigma^+)$ to $NH(A^3\Pi)$: Gateway-Mediated and Direct Mechanisms," *J. Chem. Phys.* 111, 4598-4612 (1999).	NH(a,b/A) E-E Transfer Collision Induced Cross Sections Measurements
(82958)	Rydberg State Autoionization, Electric Field Effects, Analysis	NO Predissociation
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(83215)	Predissociation, Na, $H_2(v,J)$ Product Channel, Reaction Dynamics	$NaH_2(A)$
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(83217)	Reaction Probabilities, ClO(v) Product, Calculations	$O(^1D)+HCl(v)$
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(83267)	P.E. Surfaces, Construction Methods, Review	$O(^1D)+H_2$ OH(A).Ar

(83223)	Crossed Beam Scattering, Reaction Dynamics, Overview	$O(^1D),N(^2D),S(^1D)+H_2$
(83169)	OH(v,J) Product Energies, Comparisons, Dynamics	$O(^1D)+H_2O,D_2O$ $O(^1D)+(H_2O)_n,(D_2O)_n$ $N_2O/H_2O,D_2O+h\nu$
(83162) (83163)	NO(v,J) Product Energy Distributions, Two NO Product Differences, Cross Sections, Product Vector Properties	$O(^1D)+N_2O$
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(83168)	Quenching Rate Constants, Measurements	$OH(A,v=0,N)+O_3$
(83292)	Rydberg/Valence (6.5-9.5 eV Energy), Predissociations, Assignments, P.E. Curves, Analysis	$O_2(^{1,3}\Pi_g)$
(82969)	Perturbations, Interacting States, Analysis	$O_2(d^1\Pi_g/C^3\Pi_g)$
(83264)	Perturbation Analysis, Measurements	$O_2(b,v=19/X,v=28)$
(83172)	P.E. Surfaces, Transition State, Dynamics	$^1O_2+(CH_3)_2S$
(82975)	R2PI Spectra, State Assignments, Constants, Lifetimes	PdC*
(83220)	Reaction Dynamics, Channels, Reactivities	$Pt^*,Pt+C_2H_4$ $Pd^*,Pd+C_2H_4$
(83295)	Low-lying States, Lifetimes, P.E. Curves, Spectral Constants, D_e, T_e, Calculations	SiO^+
83014.	Alekseev, V.A., and D.W. Setser, "Generation and Kinetic Studies of $Xe(5d[3/2]_1)$ Resonance State Atoms," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 8396-8403 (1999).	$Xe(5d_{1/2})+M$ Quenching Rate Constants 10 Reactants
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28. FRANCK-CONDON FACTORS/TRANSITION PROBABILITIES

(See also Section 27 for Lifetimes and Transition Probabilities)

(82901)	Transition Probabilities, Absorption Spectra, ^{1,3}Energy Splitting, Measurements	Ar_2(5p-4s)
(83269)	F.C. Factors, P.E. Curves, Spectral Constants, Calculations	CP(A-X)
(83307)	Oscillator Strengths, Low-lying States, Structural Calculations, Frequencies, Energies	*c*-C_4H_5N
(82926)	Oscillator Strength Calculations, Electronic Absorption Spectra	C_n
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(82954)	LIF Spectra, Line Polarizations/Grating Interaction Potential Effects, $Li_2(1^3\Sigma_g^-,1^3\Delta_g\text{-}1(b)^3\Pi_u)$	Line Intensities
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(82914)	Infrared Band Strengths, FTIR Spectrum, Assignments, Frequencies	CF_3CHFI
(83332)	Line Broadening Coefficients, Rotational Energy Transfer, Calculations	C_2H_2(J)+He
(83096)	Infrared Band Intensities	$CHF_2OCF_2OCHF_2$ $CHF_2O(CF_2)_2OCHF_2$ $CHF_2O(CF_2)_2OCF_2OCHF_2$ $CH_3OC_4F_9$

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(83312) Infrared Intensities, Structural Calculations, Frequencies — NH_2(B,A,X)

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(83314) Infrared Intensities, Dipole Moments, Structural Calculations, Geometries, Frequencies — HSiSiO(A,X)

30. ANALYSIS/MONITORING TECHNIQUES

(82706) Explosives, Energetic Materials, Review — Detection Methods

(82737) Atmospheric Pressure Monitor, Ionizer, HOCl Measurements — Mass Spectrometry

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31. FLAME CONCENTRATION MEASUREMENTS

(See also Section 34 for Flame Species Profiles)

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83049.	Bakali, A.E., J.-L. Delfau and C. Vovelle, "Experimental Study of Atmospheric Pressure, Rich, Premixed *n*-Heptane and *iso*-Octane Flames," *Combust. Sci. Technol.* 140, 69-91 (1998).	Species Profiles *n*-$C_7H_{16}/O_2/N_2$ *i*-$C_8H_{18}/O_2/N_2$ GC/MS Analysis Flame Structure
83050.	Korobeinichev, O.P., S.B. Ilyin, V.M. Shvartsberg and A.A. Chernov, "The Destruction Chemistry of Organophosphorus Compounds in Flames. I. Quantitative Determination of Final Phosphorus-Containing Species in Hydrogen/Oxygen Flames," *Combust. Flame* 118, 718-726 (1999).	Species Profiles PO,PO_2 HOPO,$HOPO_2$ H_2/O_2/P Mass Analysis Calibrations
83051.	Korobeinichev, O.P., V.M. Shvartsberg and A.A. Chernov, "The Destruction Chemistry of Organophosphorus Compounds in Flames. II. Structure of a Hydrogen/Oxygen Flame Doped with Trimethyl Phosphate," *Combust. Flame* 118, 727-732 (1999).	Species Profiles PO,PO_2 HOPO,$HOPO_2$ H_2/O_2/P Mass Analysis Mechanisms

32. MAPPING/TOMOGRAPHIC METHODS

(82667)	Surface Orientation, Turbulent Premixed Flames, Measurements	Laser Tomography
(83158)	Fragment Imaging, $D_2+h\nu$	D^+,e^-
(83166)	Product Velocity Imaging Method, $O_2+h\nu$	$O(^3P_J)$
(82688)	Predissociative O_2 LIF, Turbulent H_2/Liquid O_2 Coaxial Jet	2-D Imaging

33. OPTOGALVANIC/OPTOACOUSTIC METHODS

83052.	Harren, F.J.M., J. Oomens, S. Persijn, R.H. Veltman, H.S.M. de Vries and D.H. Parker, "Multi-Component Trace Gas Analysis with a CO Laser Based Photoacoustic Detector: Emission of Ethanol, Acetaldehyde, Ethane and Ethylene from Fruit," in *ROMOPTO '97: Fifth Conference on Optics*, V.I. Vlad and D.C. Dumitras, eds., 184 Papers Presented at a Conference Held in Bucharest, Romania, September 1997, 1228 pp., Published in 2 Volumes, Volume 1, pp. 1-639, *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3405, 556-562 (1998).	C_2H_5OH,C_2H_4 C_2H_6,CH_3CHO Optoacoustic Monitor
(83036)	Optogalvanic Monitor, Diode Laser Absorption, Frequency Modulation, Xe/Ne Discharge	$Xe(1s_4)$

34. FLAME KINETIC MODELING

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(82839)	Reduced Kinetics, Modeling, NO_x Formation, Heat Release, New Methodology	CH_4/Air
83054.	Massias, A., D. Diamantis, E. Mastorakos and D.A. Goussis, "Global Reduced Mechanisms for Methane and Hydrogen Combustion with Nitric Oxide Formation Constructed with Computational Singular Perturbation Data," *Combust. Theory Modeling* 3, 233-257 (1999).	Kinetic Modeling CH_4,H_2/Air Reduced Scheme NO Formation Adequacies
83055.	Davis, S.G., C.K. Law and H. Wang, "Propene Pyrolysis and Oxidation Kinetics in a Flow Reactor and Laminar Flames," *Combust. Flame* 119, 375-399 (1999).	Kinetic Modeling C_3H_6 Pyrolysis C_3H_6/O_2 Species Profiles C_3H_6/Air Flame Speeds Uncertainties

83056.	Dagaut, P., and M. Cathonnet, "The Oxidation of 1,3-Butadiene: Experimental Results and Kinetic Modeling," *Combust. Sci. Technol.* 140, 225-257 (1998).	Kinetic Modeling C_4H_6/O_2 Jet Stirred Reactor Species Profiles Probe/GC Major Channels
83057.	Dagaut, P., and M. Cathonnet, "Isobutene Oxidation and Ignition: Experimental and Detailed Kinetic Modeling Study," *Combust. Sci. Technol.* 137, 237-275 (1998).	Kinetic Modeling i-C_4H_8/O_2 Jet Stirred Reactor Species Profiles Probe Sampling
83058.	Voisin, D., A. Marchal, M. Reuillon, J.-C. Boettner and M. Cathonnet, "Experimental and Kinetic Modeling Study of Cyclohexane Oxidation in a Jet Stirred Reactor at High Pressure," *Combust. Sci. Technol.* 138, 137-158 (1998).	Kinetic Modeling c-C_6H_{12}/O_2 Stirred Reactor 10 atm,750-1100 K Species Profiles
83059.	Olsen, R.J., and D.G. Vlachos, "A Complete Pressure-Temperature Diagram for Air Oxidation of Hydrogen in a Continuous-Flow Stirred Tank Reactor," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7990-7999 (1999).	Kinetic Modeling H_2/Air Stirred Reactor P,T Dependence Oscillatory Behavior

35. PYROLYSIS KINETICS/STUDIES

83060.	Arenas, J.F., J.I. Marcos, J.C. Otero, A. Sanchez-Galvez and J. Soto, "A Multiconfigurational Self-Consistent Field Study of the Thermal Decomposition of Methyl Azide," *J. Chem. Phys.* 111, 551-561 (1999).	Pyrolysis CH_3N_3 Channels Energy Barriers Reaction Dynamics
(83055)	Pyrolysis, Species Profiles, Kinetic Modeling, Flow Reactor	C_3H_6
83061.	Gladky, A.Yu, V.K. Ermolaev and V.N. Parmon, "Temperature Dependence of Chain Initiation in Pyrolysis of Propane Studied by Direct Mass Spectrometric Detection of Methyl Radicals," *React. Kinet. Catal. Lett.* 67, 183-189 (1999).	Pyrolysis C_3H_8 CH_3 Monitoring Mass Analysis
83062.	Dorge, K.J., D. Tanke and H.G. Wagner, "Particle Formation in Carbon Suboxide Pyrolysis behind Shock Waves," *Z. Phys. Chem. (Munchen)* 212, 219-229 (1999).	Pyrolysis C_3O_2/Ar Soot Formation Shock Tube Yield,Sizes

83063. Zegers, E.J.P., and E.M. Fisher, "Pyrolysis of Triethyl Phosphate," *Combust. Sci. Technol.* 138, 85-103 (1998).

Pyrolysis
$(C_2H_5)_3PO_4$
Product Analysis
Unimolecular
Rate Parameters

83064. Stewart, J., K. Brezinsky and I. Glassman, "Supercritical Pyrolysis of Decalin, Tetralin and *n*-Decane at 700-800 K: Product Distribution and Reaction Mechanism," *Combust. Sci. Technol.* 136, 373-390 (1998).

Pyrolysis
$C_{10}H_{10}$,$C_{10}H_{12}$
n-$C_{10}H_{22}$
Flow Reactor
Major Products

83065. Singh, G., I.P.S. Kapoor, S.M. Mannan and S.K. Tiwari, "Studies on Energetic Compounds. XI. Preparation and Thermolysis of Polynitro-Organic Compounds," *J. Hazardous Mat.* A68, 155-178 (1999).

Pyrolysis
Polynitro-organics
Review

36. KINETIC MODELING/SENSITIVITIES/RATE CONSTANTS

(See also Section 15 for Ion Reaction Rate Constants, Section 27 for Excited State Rate Constants, Section 39 for Unimolecular Rate Constants, Section 40 for Theoretically Calculated Values and Section 45 for Energy Relaxation Rate Constants)

83066. Najm, H.N., P.S. Wyckoff and O.M. Knio, "A Semi-Implicit Numerical Scheme for Reacting Flow. I. Stiff Chemistry," *J. Computat. Phys.* 143, 381-402 (1998).

Kinetic Modeling
2-D Unsteady
Combustion
Integration Method

83067. Knio, O.M., H.N. Najm and P.S. Wyckoff, "A Semi-Implicit Numerical Scheme for Reacting Flow. II. Stiff, Operator-Split Formulation," *J. Computat. Phys.* 154, 428-467 (1999).

Kinetic Modeling
2-D Unsteady
Combustion
Stiff Integrator
Method

83068. Heard, A.C., M.J. Pilling and A.S. Tomlin, "Mechanism Reduction Techniques Applied to Tropospheric Chemistry," *Atm. Environ.* 32, 1059-1073 (1998).

Kinetic Modeling
Tropospheric
Chemistry
Reduction
Techniques

(82780) Oscillatory Solutions, Tropospheric Chemistry, CO, NO, O_3 Controlling Parameters

Kinetic Modeling

83069. Shorter, J.A., P.C. Ip and H.A. Rabitz, "An Efficient Chemical Kinetics Solver Using High Dimensional Model Representation," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7192-7198 (1999).

Kinetic Modeling
Computational
Acceleration
Stratospheric
Chemistry
Accuracies

83070. Capitelli, M., I. Armenise and C. Gorse, "State-to-State Approach in the Kinetics of Air Components Under Re-entry Conditions," *J. Thermophys. Heat Transfer* 11, 570-578 (1997).

Kinetic Modeling
Air
Hypersonic Flows
$N_2(v)$ Nonequilibrium Effects
NO Formation

83071. Ingham, T., D. Bauer, R. Sander, P.J. Crutzen and J.N. Crowley, "Kinetics and Products of the Reactions BrO+DMS and Br+DMS at 298 K, where DMS is Dimethyl Sulfide," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7199-7209 (1999).

$Br+(CH_3)_2S$
$BrO+(CH_3)_2S$
Rate Constants
Products
Mechanism

83072. Husain, D., and A.X. Ioannou, "Collisional Removal of Atomic Carbon, $C[2p^2(^3P_J)]$, by Aldehydes and Ketones, Investigated by Time-Resolved Atomic Resonance Absorption Spectroscopy in the Vacuum Ultraviolet," *J. Photochem. Photobiol. A. Chem.* 129, 1-7 (1999).

C+RCHO
C+RCOR′
10 Rate Constants
Rapid Reactions

83073. Caballero, N.B., E. Castellano, C.J. Cobos, A.E. Croce and G.A. Pino, "Kinetics of the Recombination Reactions of CClF with CF_2 and with CClF," *Chem. Phys.* 246, 157-166 (1999).

$CClF+CF_2+M$
CClF+CClF+M
Rate Constants
Measurements
$\Delta H_f(C_2ClF_2)$
$\Delta H_f(C_2Cl_2F_2, C_2F_3)$
Calculations

83074. Czarnowski, J., "Kinetics and Mechanisms of the Thermal Gas Phase Reactions of CF_3OF and CF_3OOCF_3 with NO_2," *Z. Phys. Chem. (Munchen)* 210, 83-94 (1999).

CF_3OF+NO_2
$(CF_3O)_2+NO_2$
CF_3O+NO_2
Rate Constants
P,T Dependences
Products

83075. Bergeat, A., T. Calvo, G. Dorthe and J.-C. Loison, "Fast-Flow Study of the CH+CH Reaction Products," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6360-6365 (1999).

CH+CH
Branching Ratios
$C_2H(A), C_2(d)$
Chemiluminescence
Measurements

83076. Fahr, A., A.H. Laufer and D.C. Tardy, "Pressure Effect on CH_3 and C_2H_3 Cross-Radical Reactions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 8433-8439 (1999).

$CH_3+C_2H_3+M$
Rate Constants
Pressure Effects
Measurements

83077. Krasnoperov, L.N., and K. Mehta, "Kinetic Study of CH_3+HBr and CH_3+Br Reactions by Laser Photolysis-Transient Absorption over 1-100 Bar Pressure Range," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 8008-8020 (1999).

CH_3+HBr
CH_3+Br
Rate Constants
P Dependences
$(CH_3)_2CO+h\nu$
CH_3CO Yields

83078. Butkovskaya, N.I., and D.W. Setser, "Product Branching Fractions and Kinetic Isotope Effects for the Reactions of OH and OD Radicals with CH_3SH and CH_3SD," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6921-6929 (1999).

CH_3SH+OH,OD
CH_3SD+OH,OD
Branching Ratios
Isotope Effects

83079. Hessler, J.P., "New Empirical Rate Expression for Reactions without a Barrier: Analysis of the Reaction of CN with O_2," *J. Chem. Phys.* 111, 4068-4076 (1999).

$CN+O_2$
Negative Temperature Expression
Rate Constant Analysis

83080. Thuner, L.P., I. Barnes, K.H. Becker, T.J. Wallington, L.K. Christensen, J.J. Orlando and B. Ramacher, "Atmospheric Chemistry of Tetrachloroethene ($Cl_2C=CCl_2$): Products of Chlorine Atom Initiated Oxidation," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 8657-8663 (1999).

C_2Cl_4+Cl
Rate Constants
Fall-off Parameters
$C_2Cl_4/O_2(NO_x)$
Product Yields
$COCl_2$,CCl_3COCl
Mechanism

83081. Acerboni, G., N.R. Jensen, B. Rindone and J. Hjorth, "Kinetics and Products Formation of the Gas Phase Reactions of Tetrafluoroethylene with OH and NO_3 Radicals and Ozone," *Chem. Phys. Lett.* 309, 364-368 (1999).

C_2F_4+OH,O_3
$C_2F_4+NO_3$
Rate Constants
COF_2 Product
Atmospheric Lifetime

83082. Zhu, L., J.W. Bozzelli and W.-P. Ho, "Reaction of OH Radical with C_2H_3Cl: Rate Constant and Reaction Pathway Analysis," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7800-7810 (1999).

C_2H_3Cl+OH
Rate Constants
Branching Ratios
Kinetic Analysis

83083. Moise, T., W. Denzer and Y. Rudich, "Direct Kinetics Study of the Reaction of Peroxyacetyl Radical with NO between 218 and 370 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6766-6771 (1999).

$CH_3C(O)O_2+NO$
Rate Constants
T Dependence
Measurements

83084. Atkinson, D.B., and J.W. Hudgens, "Chorination Chemistry. I. Rate Coefficients, Reaction Mechanisms and Spectra of the Chlorine and Bromine Adducts of Propargyl Halides," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7978-7989 (1999).

C_3H_3Cl+Cl
C_3H_3Br+Br
$C_3H_3Cl_2+C_3H_3Cl_2$
$C_3H_3Br_2+C_3H_3Br_2$
Rate Constants
$C_3H_3Cl_2$,C_3H_3ClBr
$C_3H_3Br_2$
Absorption Cross Sections

83085. Grosjean, E., and D. Grosjean, "The Reaction of Unsaturated Aliphatic Oxygenates with Ozone," *J. Atm. Chem.* 32, 205-232 (1999).

$RH + O_3$
6 Oxygenated Unsaturated Organics
Rate Constants
Major Products

83086. Wang, J.J., and L.F. Keyser, "Kinetics of the $Cl(^2P_J) + CH_4$ Reaction: Effects of Secondary Chemistry below 300 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7460-7469 (1999).

$Cl + CH_4$
Rate Constants
T Dependence
Measurements

83087. Fernandez-Alonso, F., B.D. Bean and R.N. Zare, "Measurement of the $HD(v'=2,J'=3)$ Product Differential Cross Section for the $H + D_2$ Exchange Reaction at 1.55(±0.05) eV Using the Photoloc Technique," *J. Chem. Phys.* 111, 1022-1034 (1999).

$H + D_2$
1.55 eV Energy
Product $HD(v=2,J=3)$
Cross Sections
New System

83088. Fernandez-Alonso, F., B.D. Bean and R.N. Zare, " Differential Cross Sections for $H + D_2 \rightarrow HD(v'=1,J'=1,5,8) + D$ at 1.7 eV," *J. Chem. Phys.* 111, 1035-1042 (1999).

$H + D_2$
1.7 eV Energy
Product $HD(v=1,J=1,5,8)$
Cross Sections
Measurements

83089. Fernandez-Alonso, F., B.D. Bean and R.N. Zare, "Differential Cross Sections for $H + D_2 \rightarrow HD(v'=2,J'=0,3,5) + D$ at 1.55 eV," *J. Chem. Phys.* 111, 2490-2498 (1999).

$H + D_2$
1.55 eV Energy
$HD(v=2,J=0,3,5)$
Product
Cross Sections
Measurements

83090. Tokos, J.J.S., B. Hall, J.A. Calhoun and E.M. Prestbo, "Homogeneous Gas Phase Reaction of Hg^0 with H_2O_2, O_3, CH_3I and $(CH_3)_2S$: Implications for Atmospheric Hg Cycling," *Atm. Environ.* 32, 823-827 (1998).

$Hg + H_2O_2$
Rate Constant
$Hg + CH_3I$
$Hg + (CH_3)_2S, O_3$
Atmospheric Roles

83091. Campbell, M.L., "Temperature Dependent Rate Constants for the Reactions of Gas Phase Lanthanides with N_2O," *J. Chem. Phys.* 111, 562-566 (1999).

$Ln + N_2O$
Ln = La thru Yb
Rate Constants
T Dependences
Measurements

83092. Campbell, M.L., "Temperature Dependent Rate Constants for the Reactions of Gas Phase Lanthanides with O_2," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7274-7279 (1999).

$Ln + O_2$
Ln = La thru Yb
Rate Constants
T Dependences

83093. Moonen, P.C., J.N. Cape, R.L. Storeton-West and R. McColm, "Measurement of the $NO+O_3$ Reaction Rate at Atmospheric Pressure Using Realistic Mixing Ratios," *J. Atm. Chem.* 29, 299-314 (1998).

$NO+O_3$(Air)
Rate Constants
P,T Dependences
Low Mixing Ratios

83094. Mauersberger, K., B. Erbacher, D. Krankowsky, J. Gunther and R. Nickel, "Ozone Isotope Enrichment: Isotopomer-Specific Rate Coefficients," *Science* 283, 370-372 (1999).

$O+O_2+M$
Rate Constants
6 Isotopic Contributions
O_3 Enrichment

83095. Heathfield, A.E., C. Anastasi, P. Pagsberg and A. McCulloch, "Atmospheric Lifetimes of Selected Fluorinated Ether Compounds," *Atm. Environ.* 32, 711-717 (1998).

OH+Ethers
Rate Constants
13 Ethers
Atmospheric Lifetimes

83096. Cavalli, F., M. Glasius, J. Hjorth, B. Rindone and N.R. Jensen, "Atmospheric Lifetimes, Infrared Spectra and Degradation Products of a Series of Hydrofluoroethers," *Atm. Environ.* 32, 3767-3773 (1998).

OH+ROR′
4 Hydrofluoroethers
Rate Constants
IR Band Intensities
Products

83097. Kompitsas, M., A. Mellouki, G. Le Bras, F. Roubani-Kalantzopoulou, A. Mavropoulos and I. Bassiotis, "Kinetics of Gas Phase Tropospheric Reactions of Organic Solvents and Hydroxyl Radical by Laser Photolysis-Laser Induced Fluorescence," in *Second Greek/Italian International Conference on New Laser Technologies and Applications*, A. Carabelas, P. Di Lazzaro, A. Torre and G. Baldacchini, eds., Proceedings of a Conference Held in Olympia, Greece, June 1997, 86 Papers, 466 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3423, 271-275 (1998).

$OH+c\text{-}C_4H_8O_2$
Rate Constant Measurement

83098. Brubaker Jr, W.W., and R.A. Hites, "OH Reaction Kinetics of Gas Phase α- and γ-Hexachlorocyclohexane and Hexachlorobenzene," *Environ. Sci. Technol.* 32, 766-769 (1998).

$OH+c\text{-}C_6H_6Cl_6$
$OH+C_6Cl_6$
Rate Constants
Atmospheric Lifetimes

83099. Lipson, J.B., T.W. Beiderhase, L.T. Molina, M.J. Molina and M. Olzmann, "Production of HCl in the OH+ClO Reaction: Laboratory Measurements and Statistical Rate Theory Calculations," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6540-6551 (1999).

OH+ClO
HCl Product
Minor Branching Ratio
Rate Constants

83100. Bedjanian, Y., V. Riffault, G. Le Bras and G. Poulet, "Kinetic Study of the Reactions of OH and OD with HBr and DBr," *J. Photochem. Photobiol. A. Chem.* 128, 15-25 (1999).

OH+HBr,DBr
OD+HBr,DBr
Rate Constants
T Dependences
Reaction/ Isotope Exchange Channels

83101. Bedjanian, Y., G. Le Bras and G. Poulet, "Kinetic Study of OH+OH and OD+OD Reactions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7017-7025 (1999).

OH+OH
OD+OD
OH+OD
$D+NO_2$
Rate Constants
T Dependences
Measurements

83102. Herndon, S.C., K.D. Froyd, E.R. Lovejoy and A.R. Ravishankara, "How Rapidly Does the SH Radical React with N_2O?," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6778-6785 (1999).

$SH+N_2O$
Rate Constant
Measurement

37. PHOTOLYSIS/MPD

(See also Section 38 for Photolytic Product Distributions)

83103. Almond, M.J., "Matrix Isolation," *Ann. Repts. Prog. Chem. C. Phys. Chem.* 93, 3-55 (1997).

Photochemistry
Dissociation
Energy Transfer
Matrix Isolation
Methods
Review

83104. Bondybey, V.E., M. Rasanen and A. Lammers, "Rare Gas Matrices, Their Photochemistry and Dynamics: Recent Advances in Selected Areas," *Ann. Repts. Prog. Chem. C. Phys. Chem.* 95, 331-372 (1999).

Photochemistry
Dissociation
Energy Transfer
Matrix Isolation
Methods
Review

83105. Machholm, M., and N.E. Henriksen, "Two-Pulse Laser Control for Selective Photofragment Orientation," *J. Chem. Phys.* 111, 3051-3057 (1999).

MPD
Diatomics
Fragment
Angular
Distribution
2-Pulse Laser
Control

83106. Lin, J.T., T.L. Lai, D.S. Chuu and T.F. Jiang, "Quantum Dynamics of a Diatomic Molecule under Chirped Laser Pulses," *J. Phys. B. At. Mol. Opt. Phys.* 31, L117-L126 (1998).

MPD
Diatomics
Chirped Laser
Pulse Mode
Efficiencies

83107. Levis, R.J., and M.J. DeWitt, "Photoexcitation, Ionization and Dissociative of Molecules Using Intense Near-Infrared Radiation of Femtosecond Duration," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6493-6507 (1999).

fs IR MPD/MPI
Polyatomics
Mechanisms
Review

83108. Skowronek, S., J.B. Jimenez and A.G. Urena, "Resonances in the Ba...FCH_3+hν→BaF+CH_3 Reaction Probability," *J. Chem. Phys.* 111, 460-463 (1999).

Ba.FCH_3+hν
Dissociation
Probabilities
Transition State
Spectroscopy

83109. Franks, K.J., H. Li and W. Kong, "Evidence of a Perpendicular Component in the Photodissociation of BrCN at 213 nm," *J. Chem. Phys.* 111, 1884-1889 (1999).

BrCN+hν
Aligned Cooled
Beam
CN,LIF
Fragment
Polarizations

83110. Loock, H.-P., J. Cao, W.J. Balfour, C. Zhou and C.X.W. Qian, "Spectroscopy and Dynamics Involving Interacting Electronic States," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 47-50 (1998).

BrCl+hν
BrNO+hν
Fragment Energies
ReN(18.5-X)
Deperturbation
State Couplings
Dynamics

83111. Jung, Y.-J., M.S. Park, Y.S. Kim, K.-H. Jung, H.-R. Volpp, "Photodissociation of $CBrCl_3$ at 234 and 265 nm: Evidence of the Curve Crossing," *J. Chem. Phys.* 111, 4005-4012 (1999).

$CBrCl_3$+hν
Br($^2P_{1/2,3/2}$)
Product
Quantum Yields
Dynamics

83112. Suh, M., W. Sung, S.-U. Heo and H.J. Hwang, "Energy Relaxation Dynamics of Photofragments Measured by Probe Beam Deflection Technique: Photodissociation of CF_3I at 266 nm," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 8365-8371 (1999).

CF_3I+hν
Fragment Energy
Relaxation
CF_3(T,v)+Ar
Rates
Measurements

83113. Waugh, S.E., A.C. Terentis, G.F. Metha and S.H. Kable, "On the Conservation of Angular Momentum in Polyatomic Photochemical Reactions: $H_2CO(v,J,K_a,K_c) \rightarrow H+HCO(N,K_a,K_c,J)$," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 36-46 (1998).

CH_2O+hν
HCO Product
Energies
Dynamics

83114. Kosmidis, C., K.W.D. Ledingham, H.S. Kilic, T. McCanny, R.P. Singhal, D. Smith and A.J. Langley, "Molecular Fragmentation Induced by Femtosecond Laser," in *Second Greek/Italian International Conference on New Laser Technologies and Applications*, A. Carabelas, P. Di Lazzaro, A. Torre and G. Baldacchini, eds., Proceedings of a Conference Held in Olympia, Greece, June 1997, 86 Papers, 466 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3423, 204-208 (1998).

MPD
CH_3NO_2,$C_6H_5NO_2$
$C_6H_4(NO_2)CH_3$
fs Pulsed Laser
Product Fragment
Mass Analysis

83115. Harich, S., J.J. Lin, Y.T. Lee and X. Yang, "Competing Atomic and Molecular Hydrogen Pathways in the Photodissociation of Methanol at 157 nm," *J. Chem. Phys.* 111, 5-9 (1999).

$CH_3OH + h\nu$
D Isotopes
H Loss Channels
H/H_2 Loss
Branching Ratio

83116. Ungureanu, C., and M. Ungureanu, "Infrared Photochemistry of Trichloroethylene in Presence of Oxygen," in *ROMOPTO '97: Fifth Conference on Optics*, V.I. Vlad and D.C. Dumitras, eds., 184 Papers Presented at a Conference Held in Bucharest, Romania, September 1997, 1228 pp., Published in 2 Volumes, Volume 1, pp. 1-639, *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3405, 596-602 (1998).

IR MPD
C_2HCl_3/O_2
Product
Mass Analysis

83117. Schmid, R.P., Y. Ganot, T. Arusi-Parpar, R.-J. Li, I. Bar and S. Rosenwaks, "State-Selective Dissociation of Acetylene Isotopomers," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 28-35 (1998).

$C_2HD(5\nu_{CH}) + h\nu$
$C_2H_2(v) + h\nu$
Overtone
Dissociation
H,D Product
Branching

83118. Ashikhmin, M.V., A. Mellinger and C.B. Moore, "The Photodissociation of Singlet Ketene by Two-Step Infrared Plus Ultraviolet Excitation," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 64-70 (1998).

$CH_2CO + h\nu$
CH_2
Product Energies
Dynamics

83119. Drabbels, M., C. Morgan and A.M. Wodtke, "Molecular Square Dancing: Correlated Product Motion in Photodissociation," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 51-63 (1998).

$CH_2CO + h\nu$
CH_2
Product State
Distributions
Measurements
Theoretical
Shortcomings

83120. Yarkony, D.R., "S_1-S_0 Internal Conversion in Ketene. I. The Role of Conical Intersections," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6658-6668 (1999).

$CH_2CO + h\nu$
S_1/S_0 Conversion
Conical
Intersection
Dynamics

83121. North, S.W., and G.E. Hall, "Transient Frequency-Modulated Spectroscopy: Application to the Measurement of Vector and Scalar Correlations in Molecular Photodissociation," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 95-102 (1998).

$CH_2CO + h\nu$
$ICN + h\nu$
Frequency
Modulation
Vector Correlations
$CH_2(a)$,CN

83122. Xu, K., and J. Zhang, "Photodissociation of the Vinyl Radical (C_2H_3) via the First Excited State: The $C_2H_2(X^1\Sigma_g^+)$+H Channel," *J. Chem. Phys.* 111, 3783-3786 (1999).
C_2H_3 + hν
Product
C_2H_2, H
Kinetic Energy
Distributions
D_0

83123. Suzuki, T., T. Shibata and H. Li, "Dissociation of Metastable CH_3CO Radical Studied by Time-Resolved Photofragment Imaging," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 2-6 (1998).
CH_3COCl + hν
CH_3CO Fragment
Energies
Imaging Method

83124. Deyerl, H.-J., I. Fischer and P. Chen, "Photodissociation Dynamics of the Propargyl Radical," *J. Chem. Phys.* 111, 3441-3448 (1999).
C_3H_3 + hν
H Atom
Detection
Rates
RRKM Analysis
Product Energy

83125. Mebel, A.M., W.M. Jackson, A.H.H. Chang and S.H. Lin, "Photodissociation Dynamics of Propyne and Allene: A View from ab Initio Calculations of the C_3H_n(n=1-4) Species and the Isomerization Mechanism for C_3H_2," *J. Am. Chem. Soc.* 120, 5751-5763 (1998).
C_3H_4 + hν
P.E. Surfaces
Channels
Energies
Dynamics

(83077) CH_3CO Yields, Measurements
$(CH_3)_2CO$ + hν

83126. Wu, S.M., J.J. Lin, Y.T. Lee and X. Yang, "Site Specificity in Molecular Hydrogen Elimination from Photodissociation of Propane at 157 nm," *J. Chem. Phys.* 111, 1793-1796 (1999).
C_3H_8 + hν
H_2 Elimination
Channel
Site Effects
H,H_2 Product
Branching Ratios

83127. Forde, N.R., M.L. Morton, S.L. Curry, S.J. Wrenn and L.J. Butler, "Photodissociating Trimethylamine at 193 nm to Probe Dynamics at a Conical Intersection and to Calibration Detection Efficiency of Radical Products," *J. Chem. Phys.* 111, 4558-4568 (1999).
$(CH_3)_3N$ + hν
Fragments
Velocities
Channels
Mechanisms

83128. Sorkhabi, O., F. Qi, A.H. Rizvi and A.G. Suits, "Ultraviolet Photodissociation of Furan Probed by Tunable Synchrotron Radiation," *J. Chem. Phys.* 111, 100-107 (1999).
c-C_4H_4O + hν
(193 nm)
Primary Channels
Energy Barriers
Product Angular
Distributions

83129. Qi, F., O. Sorkhabi, A.H. Rizvi and A.G. Suits, "193 nm Photodissociation of Thiophene Probed Using Synchrotron Radiation," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 8351-8358 (1999).

c-$C_4H_4S + h\nu$
Channels
Product Energies
Measurements

83130. Parker, J.K., and S.R. Davis, "Photochemical Reaction of Ozone and Dimethylacetylene: An Infrared Matrix Isolation and ab Initio Investigation," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7280-7286 (1999).

$CHC(CH_3)_2/O_3 + h\nu$
Product Analysis
Mechanism
Matrix Study

83131. Ichimura, T., "Photodissociation Dynamics of Chlorinated Benzene Derivatives," pp. 233-262 in *Structure and Dynamics of Electronic Excited States*, J. Laane, H. Takahashi and A. Bandrauk, eds., 12 Papers Presented at the Pacifichem 95 Meeting, Held in Honolulu HI, December 1995, 320 pp., Springer-Verlag, Berlin (1999).

$C_6H_5Cl, C_6F_5Cl + h\nu$
$C_6H_4Cl_2 + h\nu$
$C_6H_4(Cl)CH_3 + h\nu$
Product Energy
Partitioning
Dynamics

83132. Parker, J.K., and S.R. Davis, "Photochemical Reaction of Ozone and Benzene: An Infrared Matrix Isolation Study," *J. Am. Chem. Soc.* 121, 4271-4277 (1999).

$C_6H_6/O_3 + h\nu$
Products
Matrix Study

83133. Kumar, A., P.D. Naik, R.D. Saini and J.P. Mittal, "Direct Evidence of a Radical Channel in Photodissociation of 1,4-Cyclohexadiene with ArF Laser at 193 nm," *Chem. Phys. Lett.* 309, 191-197 (1999).

c-$C_6H_8 + h\nu$
c-C_6H_7, C_6H_6
H, H_2 Products
Channels

83134. Fuss, W., K.L. Kompa, T. Schikarski, W.E. Schmid and S.A. Trushin, "Probing of Ultrafast Photoinduced Isomerization and Dissociation Reactions by Intense-Field Dissociative Ionization," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 114-130 (1998).

MPD
c-C_6H_8, c-$C_7H_8 + h\nu$
$Cr(CO)_6 + h\nu$
fs Dynamics
Internal
Conversions

83135. Hwang, D.W., J.J. Lin, Y.T. Lee and X. Yang, "Vacuum Ultraviolet Photodissociation Dynamics of OClO: Binary and Triple Dissociation," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 15-25 (1998).

$ClO_2 + h\nu$
Branching Ratio
Binary,Triple
Product Channels

83136. Ashfold, M.N.R., P.A. Cook, S.R. Langford, A.J. Orr-Ewing and P.M. Regan, "Near Ultraviolet Photodissociation Dynamics of HBr and HI Revealed by H (Rydberg) Atom Photofragment Translational Spectroscopy," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 84-94 (1998).

$HBr + h\nu$
$HI + h\nu$
$Br, I(^2P_{1/2,3/2})$
Branching Ratios
Dynamics

83137.	Borges Jr, I., G. Jalbert and C.E. Bielschowsky, "Photon and Electron Impact Dissociation Cross Sections of HCl," *J. Phys. B. At. Mol. Opt. Phys.* 31, 3703-3711 (1998).	HCl Photodissociation e^- Impact Cross Sections Calculations
83138.	Juanes-Marcos, J.C., and A. Garcia-Vela, "Photodissociation of Ar-HCl: An Energy Resolved Study of the Dynamics of Total Fragmentation into H+Ar+Cl," *J. Chem. Phys.* 111, 2606-2619 (1999).	HCl.Ar+hν UV Photolysis H,Cl,Ar Fragments Channel Wavepacket Treatment
83139.	Kaledin, A.L., Q. Cui, M.C. Heaven and K. Morokuma, "Ab Initio Theoretical Studies on Photodissociation of HNCO upon $S_1(^1A'')\leftarrow S_0(^1A')$ Excitation: The Role of Internal Conversion and Intersystem Crossing," *J. Chem. Phys.* 111, 5004-5016 (1999).	HNCO+hν Photodissociation Dynamics Channels Calculations
83140.	Zhang, J., K. Xu and G. Amaral, "Photodissociation of HN_3 at 248 nm," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 271-279 (1998).	HN_3+hν H,N_3 Product Distributions Dynamics $D_0(HN_3)$
83141.	Minaev, B.F., "The Singlet-Triplet Absorption and Photodissociation of the HOCl, HOBr and HOI Molecules Calculated by the MCSCF Quadratic Response Method," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7294-7309 (1999).	HOCl+hν HOBr,HOI ^{1,3}Absorption Strengths Contributions Calculations
83142.	Atabek, O., C. Dion and A. Keller, "Alignment in Angular Resolved Multiphoton Spectra of H_2^+," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 262-270 (1998).	MPD H_2^+ Fragment Alignments Calculations
83143.	Volkova, E.A., A.M. Popov and O.V. Tikhonova, "Dissociation of Molecular Hydrogen Ions by an Infrared Laser Pulse," *J. Exp. Theoret. Phys.* 86, 71-78 (1998).	IR MPD H_2^+,D_2^+,HD^+ Probabilities Numerical Modeling
83144.	Rottke, H., C. Trump and W. Sandner, "Multiphoton Ionization and Dissociation of H_2O," *J. Phys. B. At. Mol. Opt. Phys.* 31, 1083-1096 (1998).	MPD/MPI H_2O Product Ions H^+,H_2^+,O^+,OH^+ Mechanism

83145. Liu, X., D.W. Hwang, X.F. Yang, S. Harich, J.J. Lin and X. Yang, "Photodissociation of Hydrogen Sulfide at 157.6 nm: Observation of SH Bimodal Rotational Distribution," *J. Chem. Phys.* 111, 3940-3945 (1999).

$H_2S+h\nu$
H,SH(v,J)
Product Energies
Two Channels

83146. Wrenn, S.J., L.J. Butler, G.A. Rowland, C.J.H. Knox and L.F. Phillips, "The Necessity for Multiphoton Processes in the 193 nm Photochemistry of Sulfuric Acid Aerosols," *J. Photochem. Photobiol. A. Chem.* 129, 101-104 (1999).

H_2SO_4 Aerosol$+h\nu$
Impurity Effects
Multiphoton
Process

83147. Radi, P.P., P. Beaud, D. Franzke, H.-M. Frey, T. Gerber, B. Mischler and A.-P. Tzannis, "Femtosecond Photoionization of $(H_2O)_n$ and $(D_2O)_n$ Clusters," *J. Chem. Phys.* 111, 512-518 (1999).

$(H_2O)_n+h\nu$
$(D_2O)_n+h\nu$
fs Photoionization
Protonated Product
Cluster Ions
Unimolecular
Dissociations

83148. Efthimiopoulos, T., D. Zevgolis, J. Katsenos and D. Zigos, "A Study of the Laser Action from HgBr($B^2\Sigma$-$X^2\Sigma$) Induced by Ultraviolet Laser Multiphoton Dissociation of $HgBr_2$: Measurements and Experimental Results," in *Second Greek/Italian International Conference on New Laser Technologies and Applications*, A. Carabelas, P. Di Lazzaro, A. Torre and G. Baldacchini, eds., Proceedings of a Conference Held in Olympia, Greece, June 1997, 86 Papers, 466 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3423, 68-71 (1998).

MPD
$HgBr_2$
Laser Emission
HgBr(B-X)

83149. Ooe, H., Y. Kimura, M. Terazima and N. Hirota, "Photodissociation Quantum Yield of Iodine in the Low-, Medium- and High-Density Fluids Studied by the Transient Grating Method," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7730-7741 (1999).

$I_2+h\nu$
Gaseous,Liquid
Photodissociation
Quantum Yields
Model

83150. Zanni, M.T., B.J. Greenblatt, A.V. Davis and D.M. Neumark, "Photodissociation Dynamics of I_3^- Using Femtosecond Photoelectron Spectroscopy," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 196-207 (1998).

$I_3^-+h\nu$
fs PES
Dynamics
I_2^-,I^-
Fragments

83151. Zanni, M.T., B.J. Greenblatt, A.V. Davis and D.M. Neumark, "Photodissociation of Gas Phase I_3^- Using Femtosecond Photoelectron Spectroscopy," *J. Chem. Phys.* 111, 2991-3003 (1999).

$I_3^-+h\nu$
Photodissociation
fs Pump/Probe
I_2^-,I^- Products
Dynamics

83152. Mayor, F.S., A. Askar and H.A. Rabitz, "Quantum Fluid Dynamics in the Lagrangian Representation and Applications to Photodissociation Problems," *J. Chem. Phys.* 111, 2423-2435 (1999).

$NOCl+h\nu$
$NO_2+h\nu$
Cross Sections
Quantum Fluid Dynamic
Lagrangian
New Approach
Calculations

83153. Nee, J.B., J.C. Yang, P.C. Lee, X.Y. Wang and C.T. Kuo, "Detection of $O(^1S)$ Produced in the Photodissociation of N_2O," *J. Phys. B. At. Mol. Opt. Phys.* 31, 5175-5181 (1998).

$N_2O+h\nu$
$O(^1S)$ Formation
Measurements
XeO Emission Spectrum

83154. Hoki, K., Y. Ohtsuki, H. Kono and Y Fujimura, "Quantum Control of NaI Predissociation in Subpicosecond and Several-Picosecond Time Regimes," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6301-6308 (1999).

$NaI+h\nu$
ps Predissociation
Laser Control Schemes

83155. Haunert, G., and E. Tiemann, "Total Fragmentation of $SbCl_3$ by Multiphoton Dissociation in the Ultraviolet," *Chem. Phys.* 246, 381-390 (1999).

UV MPD
$SbCl_3$
Sb* Emission Distribution
3-Photon Process

38. REACTION PRODUCT-ENERGY DISTRIBUTIONS

(See also Section 37 for Product Distributions and Section 40 for Theoretically Calculated Reaction Product Distributions)

83156. Scheld, H.A., A. Furlan and J.R. Huber, "The Photodissociation of Carbonyl Cyanide $CO(CN)_2$ at 193 nm Studied by Photofragment Translational Energy Spectroscopy," *J. Chem. Phys.* 111, 923-930 (1999).

CN,CO
OCCN,NCCN
Product Kinetic Energies
$CO(CN)_2+h\nu$
Channels

(82997) Product Ions, $He(2^1S)+CO_2$, Penning Ionization, Cross Sections

$CO_2^+(C,B,A,X)$

(83075) Product Chemiluminescence, CH+CH Reaction, Product Branching Ratios

$C_2H(A)$,$C_2(d)$

83157. Liu, D.-K., J.-J. Chen, C.-F. Nien and K.-C. Lin, "Nascent Rotational Distribution and Energy Disposal of the CaH Product in the Reaction of $Ca(4s4p^1P_1)+H_2 \rightarrow CaH(X^2\Sigma^+)+H$," *J. Chem. Phys.* 111, 5277-5278 (1999).

CaH(v,J)
Product Energy Distributions
$Ca(^1P_1)+H_2$
Measurements

83158. Chandler, D.W., D.W. Neyer and A.J.R. Heck, "High Resolution Photoelectron Images and D^+ Photofragment Images Following 532 nm Photolysis of D_2," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 104-113 (1998).

D^+, e^-
Fragment Imaging
$D_2 + h\nu$

83159. Baumfalk, R., U. Buck, C. Frischkorn, N.H. Nahler and L. Huwel, "Photodissociation of HBr Molecules and Clusters: Anisotropy Parameters, Branching Ratios and Kinetic Energy Distributions," *J. Chem. Phys.* 111, 2595-2605 (1999).

$H, Br/Br(^2P_{1/2})$
Product Energies
Branching Ratio
$HBr + h\nu$
$(HBr)_n + h\nu$
Dynamics

(83087) (83089) Product, $H + D_2$ (1.55 eV Energy), Cross Sections, Measurements, New Experimental System

$HD(v=2, J=0,3,5)$

(83088) Product, $H + D_2$ (1.7 eV Energy), Cross Sections, Measurements

$HD(v=1, J=1,5,8)$

83160. Honma, K., and Y. Tsutsui, "Reaction Dynamics of $H + H_2S \rightarrow H(v,J) + SH$: Doppler Profiles of $H_2(B^1\Sigma_u^+ - X^1\Sigma_g^+)$," *Chem. Phys. Lett.* 309, 35-42 (1999).

$H_2(v,J)$
Product Kinetic Energies
'Hot' $H + H_2S$
Doppler Profiles

83161. Barnes, R.J., A. Sinha, P.J. Dagdigian and H.M. Lambert, "Doppler Lineshapes in the Photolysis of Laser Excited, Aligned Molecules: Application to the Vibrationally Mediated Photodissociation of HN_3," *J. Chem. Phys.* 111, 151-162 (1999).

$NH(a, N=7,10)$
Product
Doppler Profiles
$HN_3(3\nu_1) + h\nu$
Measurements
General Theory

(83004) Product Energy Distributions, $N(^2D) + CH_3OH$, CD_3OD, Mechanism

NH,OH

83162. Akagi, H., Y. Fujimura and O. Kajimoto, "Energy Partitioning in Two Kinds of NO Molecules Generated from the Reaction of $O(^1D)$ with N_2O: Vibrational State Distributions of 'New' and 'Old' NOs," *J. Chem. Phys.* 111, 115-122 (1999).

NO(v)
Product Energy Distributions
$O(^1D) + N_2O$
2 NO Product Differences
V-V Transfer

83163. Tsurumaki, H., Y. Fujimura and O. Kajimoto, "Scalar and Vector Properties of the NO(v=0) Produced from the Reaction $O(^1D) + N_2O \rightarrow NO + NO$," *J. Chem. Phys.* 111, 592-599 (1999).

$NO(v=0, T, J)$
Product Energy Distributions
$O(^1D) + N_2O$
Cross Sections
Product Vector Properties

83164.	Nestorov, V.K., and J.I. Cline, "Detection of 'Ended' NO Recoil in the 355 nm NO_2 Photodissociation Mechanism," *J. Chem. Phys.* 111, 5287-5290 (1999).	NO(X,v=0) Rotational Alignment NO_2+hν REMPI Probe
(83250)	Product Ratios, Na+Rg+hν, NaRg(B), Intermediate State, Nonadiabatic Probabilities	Na($^2P_{1/2,3/2}$)
83165.	Hsieh, C.-H., S.-H. Lee, A. Fujii and K. Liu, "Correlated Photofragmentations," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 7-14 (1998).	O(^3P_J) Product Distributions NO_2,SO_2+hν Correlation Measurements
83166.	Eppink, A.T.J.B., B. Bakker and D.H. Parker, "Velocity Imaging: Applications in Molecular Oxygen Photophysics," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 177-185 (1998).	O(^3P_J) Product Velocity Imaging Method O_2+hν
83167.	Lee, K.W., D.-C. Kim, K.-H. Jung and J.W. Hahn, "Photodissociation Dynamics of *tert*-Butyl Hydroperoxide at 213 nm via Degenerate Four-Wave Mixing Spectroscopy," *J. Chem. Phys.* 111, 1427-1432 (1999).	OH(X,v,J) Product Energy Distributions *t*-C_4H_9OOH+hν Dynamics
83168.	Dodd, J.A., R.B. Lockwood, E.S. Hwang, S.M. Miller and S.J. Lipson, "Formation of OH(v=0,1) by the Reaction of Fast H with O_3," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7834-7842 (1999).	OH(v=1,0,N) Product Energy Distributions 'Hot' H+O_3 OH(A,v=0,N)+O_3 Quenching Rate Constant
83169.	Imura, K., M. Veneziani, T. Kasai and R. Naaman, "The Reaction of O(^{1}D) with H_2O, D_2O Monomers and Clusters and the Intracomplex Reaction in N_2O-X_2O (X=H,D) Photo-initiated at 193 and 212.8 nm," *J. Chem. Phys.* 111, 4025-4031 (1999).	OH(v,J) Product Energies O(^{1}D)+H_2O,D_2O O(^{1}D)+$(H_2O)_n$,$(D_2O)_n$ N_2O/H_2O,D_2O+hν Comparisons Dynamics

39. UNIMOLECULAR PROCESSES

(See also Section 36 for Unimolecular Rate Constants and Section 40 for Reaction Dynamics)

83170.	Jursic, B.S., "High level ab Initio Computational Study of Acetylene Radical Cation and Anion Decomposition Process," *Int. J. Quantum Chem.* 72, 571-579 (1999).	Isomerization $C_2H_2^+/CCH_2^+$ $C_2H_2^-/CCH_2^-$ P.E. Surfaces Pathways
83171.	Guthe, F., R. Locht, B. Leyh, H. Baumgartel and K.-M. Weitzel, "Kinetic Energy Release Distributions in the Dissociation of Energy-Selected Fluoroethene and 1,1-Difluoroethene Ions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 8404-8412 (1999).	Unimolecular Dissociation $C_2H_3F^+$ $C_2H_2F_2^+$ Channels Measurements
83172.	McKee, M.L., "A Theoretical Study of Unimolecular Reactions of Dimethyl Persulfoxide," *J. Am. Chem. Soc.* 120, 3963-3969 (1998).	Unimolecular Dissociation $(CH_3)_2SOO$ $^1O_2 + (CH_3)_2S$ P.E. Surfaces Dynamics
83173.	Baldwin, J.E., and R. Shukla, "Thermal Isomerizations of 1,1-Dimethyl-2,2-d_2-Cyclopropane," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7821-7825 (1999).	Isomerization *c*-$C_3H_4(CH_3)_2$ D Labeling Products Mechanism
(83063)	Pyrolysis, Unimolecular Rate Parameters, Product Analysis	$(C_2H_5)_3PO_4$
83174.	Schmidt, P.P., "Hall Model Reaction Surface for HCN," *Int. J. Quantum Chem.* 72, 473-482 (1999).	Unimolecular Isomerization HCN/HNC P.E. Surface Vibrational Frequencies
83175.	Fujimura, Y., "Coherent Control of Unimolecular Reaction Dynamics Based on a Local Optimization Scheme," pp. 214-230 in *Structure and Dynamics of Electronic Excited States*, J. Laane, H. Takahashi and A. Bandrauk, eds., 12 Papers Presented at the Pacifichem 95 Meeting, Held in Honolulu HI, December 1995, 320 pp., Springer-Verlag, Berlin (1999).	Unimolecular Laser Control HCN/HNC HF$\rightarrow$ Theory

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Vibrational
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Transformation
Region

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Dissociation
HFCO + $h\nu$
ps Dynamics

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Unimolecular
Dissociation
HOCl($6\nu_{OH}$,J)
ODR Overtone
Fragment Spectra
Levels ≤300 cm^{-1}
Above Dissociation
IVR Effects

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HOCl($6\nu_{OH}$)
J Dependence
Coupling States

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Dissociation
HOCl($6\nu_{OH}$)
Interstate
Coupling/Mixing

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$(H_2O)_n + h\nu$
$(D_2O)_n + h\nu$

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NO_2
Rate Constants
P.E. Surface
IVR
Calculations

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P.E. Surface
Reaction Paths
Tunneling
Role

(See also Section 37 for Photodissociation Dynamics)

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$BrO+HO_2$

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$CHF+H$
Channels
Energies,Barriers
$\Delta H_f(CHF,CH_2F)$

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CHF_2+O
$CHCl_2+O$
Channels
Intermediates
Energies

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CHNO
P.E. Surfaces
Isomers
Pathways
Energies

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CH_3+OH
$NCO+NO$
NH_2+NO
Channels
Review

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CH_3O+CO
P.E. Surface
Channels

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CH_4/CH_3OH
Conversion
FeO^+ Catalyzed
P.E. Surfaces
Crossing Seams
Energies

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CH_4+H
Rate Constants
Tunneling Role

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$C_2H_2^+ + CH_3OH$
Channels
Energies

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Reaction Dynamics
C_2H_4+OH
Transition States
ΔH_f ,Energies
Channels
Rate Constants

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C_2H_6+H

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C_5H_8+OH
C-C Fission
Pathways
Energy Barriers

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$C_6H_5+O_2$
P.E. Surface
Channels
c-C_5H_4N,*c*-C_4H_3O
c-C_4H_3S Radicals
Comparisons

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$F+H_2$
Rate Constants
$F(^2P_{1/2})$ Contribution

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$GeXY+CH_4$
$XY=CH_2$,CH_3 ,H,
F,Cl,Br
TS Geometries
Energies

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$H+CN+Ar$
Alternate
Mechanisms

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$H+D_2(v=0,J=0)$
Vector
Correlation
Formulations

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$H+H_2$
H_2+H_2
Energy Barriers
Calculations

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$H+H_2O$
$H+D_2O$
Channels
Cross Sections
P.E. Surfaces
Inadequacies

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$HCl+O$
$HCl(v=2,J=1,6,9)+O$
New P.E. Surface
Energy Barrier
Data Comparisons

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Reaction Dynamics
$H_2^+(v)+He$
P.E. Surface
Probabilities
Channels

(82998) Reaction Dynamics, Structures, Energetics, Calculations — $Li+C_2N_2$

(82999) Reaction Dynamics, Structures, Energetics, Calculations — $Li+HCNO,HN_3,N_2O$

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$Mg(^1P_1)+H_2$
P.E. Surfaces
Product Energies
Collision Energy Effects

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P.E. Surface
Energy Barriers
Channels

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NO_2+H_2O
$N_2O_4+H_2O$
Pathways
HONO Channel
Energies

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NO_3+OH
P.E. Surfaces
Energy Barriers
Channels

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Reaction Dynamics
Na+HF
Probabilities
Attack Angle
Dependences

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NaH_2(A)
Predissociation
Na,H_2(v,J)
Product Channel

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O+HCl
J Effect Approximation
Method

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$O(^1D)$+HCl(v)
Probabilities
ClO(v′) Products
Calculations

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Reaction Dynamics
PH_2+O_2
Channels
Energetics

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Reaction Dynamics
PH_3+H
Rate Constants
Energy Barriers

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Reaction Dynamics
Pt,Pt*+C_2H_4
Pd,Pd*+C_2H_4
Channels
Reactivities

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Reaction Dynamics
SiF_4/H_2O
Intermediates
Structures
Energies

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(See also Section 42 for Laser Induced Reactions)

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Oscillatory
Kinetics
Review

(83059) H_2 /Air, Stirred Reactor, Pressure, Temperature Dependence, Kinetic Modeling | Kinetic Oscillations

(82781) Atmospheric Chemistry, Mechanistic Tool Potential | Kinetic Isotope Enrichments

83223. Casavecchia, P., N. Balucani and G.G. Volpi, "Crossed Beam Studies of Reaction Dynamics," *Ann. Rev. Phys. Chem.* 50, 347-376 (1999). | Crossed Beam Scattering
$H+H_2,D_2$
$F,Cl+H_2$
$O(^1D),N(^2D),S(^1D)+H_2$
$OH,CN+H_2$
$OH+CO$
Reaction Dynamics Overview

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Ar/CF_4
RF Discharges
Ar*(4s) Profiles
Modeling

83225. Armstrong, B.M., F. Zheng and P.B. Shevlin, "Mode of Attack of Atomic Carbon on Benzene Rings," *J. Am. Chem. Soc.* 120, 6007-6011 (1998). | $C+C_6H_6$
Reaction Products
Mechanisms

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Crossed Beams
Products
Dynamics

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C_2H_2
Products,Yields
Mass Analysis

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C_2-C_5 Alkenes
OH Product Yields

83229. Paulson, S.E., M.Y. Chung and A.S. Hasson, "OH Radical Formation from the Gas Phase Reaction of Ozone with Terminal Alkenes and the Relationship between Structure and Mechanism," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 8125-8138 (1999). | $RH+O_3$
Terminal Alkenes
OH Formation Yields

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Reactions with
NO_3,OH,O_3
Products
Mechanisms

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	Ozone: Formation Yields of Carbonyls from Biradicals in Ozone-Alkene-Cyclohexane Experiments," *Atm. Environ.* 32, 3393-3402 (1998).	Carbonyl Formation Yields Mechanisms
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83235.	Laursen, S.L., J.E. Grace Jr, R.L. DeKock and S.A. Spronk, "Reaction of NH(X) with Oxygen in a Solid Xenon Matrix: Formation and Infrared Spectrum of Imine Peroxide, HNOO," *J. Am. Chem. Soc.* 120, 12583-12594 (1998).	$NH + O_2$ HNOO Product FTIR Spectrum ^{18}O Labeling Matrix Study
83236.	Hathorn, B.C., and R.A. Marcus, "An Intramolecular Theory of the Mass-Independent Isotope Effect for Ozone. I.," *J. Chem. Phys.* 111, 4087-4100 (1999).	$O + O_2 + M/O_3 + M$ Enrichment Factors Mass Dependences Kinetic Rates Theory
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83238.	Tuazon, E.C., S.M. Aschmann, J. Arey and R. Atkinson, "Products of the Gas Phase Reactions of a Series of Methyl-Substituted Ethenes with the OH Radical," *Environ. Sci. Technol.* 32, 2106-2112 (1998).	OH + RH C_4-C_6 Alkenes Product Analysis Mechanisms
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$Y+C_2H_2,C_2D_2$
$Zr,Nb+C_2H_2$
Crossed Beams
Product Channels
Energies
D_0(Y-CCH)
Measurements

(83003) Crossed Beams, Reactivities, Energies
$Zr,V^*+C_2H_4$
Mo^*+CH_4

42. LASERS/INDUCED EFFECTS/MPI

(See also Section 26 for REMPI Spectra)

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fs Laser
Pulses
Generation
Characteristics
Spectral Usage
Reviews

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Laser Ablation
Al(s)/O_2
Al*,AlO(B-X)
Spectral Emission
Unexpected
Long Duration

(82593) Polymers, Rates
ns Laser Ablation

(82592) Polymers, Characteristics, Modeling
Laser Ablation

(82892) Lasers/Equipment, Methods, Handbook
Laser Induced
Chemistry

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Laser Control
Reactions
General Theory
Optimization
Review

(83105) Diatomic MPD, Fragment Angular Distribution
2-Pulse Laser Control

(83106) Pulse Mode Efficiencies, Diatomic MPD
Chirped Laser

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Laser Control
$(C_6H_5CH)_2$
IR/UV 2-Photon
Branching Ratio
Effects

83245. Dion, C.M., A. Keller, O. Atabek and A.D. Bandrauk, "Laser Induced Alignment Dynamics of HCN by Short, Intense Pulses," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 254-261 (1998).
Alignment
HCN
Sub ps Laser Pulses
Method

(83175) HCN/HNC, HF Dissociation, Unimolecular Processes, Theory
Laser Control

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Laser Control
HDO,H_2O
IBr,Na_2
Photodissociation
Theory

83247. Mishima, K., and K. Yamashita, "A Theoretical Study on Quantum Control of Photodissociation Dynamics by Ultrashort Chirped Laser Pulses," *Int. J. Quantum Chem.* 72, 525-532 (1999).
Reaction Control
HDO Dissociation
H,D Products
Branching Ratio
Chirped Laser
Pulse Method

83248. Posthumus, J.H., J. Plumridge, L.J. Frasinski, K. Codling, A.J. Langley and P.F. Taday, "Double Pulse Measurements of Laser Induced Alignment of Molecules," *J. Phys. B. At. Mol. Opt. Phys.* 31, L985-L993 (1998).
Laser Induced
Alignment
H_2,I_2
2-Pulse
Monitoring

83249. Brown, E.J., I. Pastirk, B.I. Grimberg, V.V. Lozovoy and M. Dantus, "Population and Coherence Control by Three-Pulse Four-Wave Mixing," *J. Chem. Phys.* 111, 3779-3782 (1999).
Laser Control
I_2
3-Pulse FWM
Population/
Coherence Transfer
Method

(83154) Laser Control Schemes, ps Predissociation
NaI+hν

83250. Grosser, J., O. Hoffmann, F.S. Wischeler and F. Rebentrost, "Direct Observation of Nonadiabatic Transitions in Na+Rare Gas Differential Optical Collisions," *J. Chem. Phys.* 111, 2853-2856 (1999).
Na+Rg+hν
NaRg(B) State
Excitation
$Na(^2P_{1/2,3/2})$
Product Ratios
Nonadiabatic
Probabilities

83251. Sukharev, M.E., and V.P. Krainov, "Rotational and Alignment of Diatomic Molecules and Their Molecular Ions in Strong Laser Fields," *J. Exp. Theoret. Phys.* 86, 318-322 (1998).
MPA/MPI
Diatomics
Rotation
Alignment
Theory

(83107)	Polyatomics, Mechanisms, Review	fs IR MPD/MPI
83252.	Sanderson, J.H., R.V. Thomas, W.A. Bryan, W.R. Newell, I.D. Williams, A.J. Langley and P.F. Taday, "High-Intensity Femtosecond Laser Interactions with Vibrationally Excited CO_2," *J. Phys. B. At. Mol. Opt. Phys.* 31, L59-L64 (1998).	fs MPI $CO_2(v)$ Vibrational Effects Interaction
83253.	Sanderson, J.H., R.V. Thomas, W.A. Bryan, W.R. Newell, A.J. Langley and P.F. Taday, "Alignment and Bending of CO_2 by Intense Femtosecond Laser Pulses," *J. Phys. B. At. Mol. Opt. Phys.* 31, L599-L606 (1998).	MPI CO_2 fs Pulses Fragment Ion Alignments
83254.	Choi, Y.-K., Y.-M. Koo and K.-W. Jung, "Multiphoton Ionization and Fragmentation Processes of Methyl Iodide Clusters at 266 and 355 nm," *J. Photochem. Photobiol. A. Chem.* 127, 1-5 (1999).	MPD/MPI $(CH_3I)_n$ Fragment Ions Mass Analysis Mechanisms
(83027)	C_6H_6, $C_6H_5CH_3$, $C_6H_5C_2H_5$, $C_6H_4(CH_3)_2$ Monitor, Detection Limits	(1+1) REMPI
83255.	Posthumus, J.H., J. Plumridge, M.K. Thomas, K. Codling, L.J. Frasinski, A.J. Langley and P.F. Taday, "Dynamic and Geometric Laser Induced Alignment of Molecules in Intense Laser Fields," *J. Phys. B. At. Mol. Opt. Phys.* 31, L553-L562 (1998).	MPD/MPI H_2,I_2,N_2 Ionic Fragment Angular Alignments
(83144)	H^+,H_2^+,O^+,OH^+ Product Ions, Mechanism, Measurements	MPD/MPI,H_2O
83256.	Kylstra, N.J., H.W. van der Hart, P.G. Burke and C.J. Joachain, "Singly, Doubly and Triply Resonant Multiphoton Processes Involving Autoionizing States in Magnesium," *J. Phys. B. At. Mol. Opt. Phys.* 31, 3089-3116 (1998).	MPI Mg Autoionizing States Excitation
(83164)	Product NO(X,v=0) Rotational Alignment, NO_2+hv, Measurements	REMPI,NO
83257.	Davies, J.A., J.E. LeClaire, R.E. Continetti and C.C. Hayden, "Femtosecond Time-Resolved Photoelectron-Photoion Coincidence Imaging Studies of Dissociation Dynamics," *J. Chem. Phys.* 111, 1-4 (1999).	MPD/MPI NO_2 fs Pump/Probe (3+1) Photon Process Mechanism
83258.	Quintella, C.M., G.G.B. de Souza and M.S.P. Mundim, "Comparative Study of Hexamethyldisiloxane Photofragmentation through Multiphotonic and Monophotonic Processes," in *Laser Techniques for State-Selected and State-to-State Chemistry IV*, J.W. Hepburn, R.E. Continetti and M.A. Johnson, eds., Proceedings of a Conference Held in San Jose CA, January 1998, 30 Papers, 288 pp., *Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.* 3271, 227-235 (1998).	MPD/MPI $(Si(CH_3)_3)_2O$ Synchrotron Light Nd.YAG Laser Product Ions Comparisons

43. P.E. CURVES/SURFACES/ENERGY LEVELS

(See also Section 26 for Spectral Aspects, Section 39 for Unimolecular P.E. Surfaces and Section 40 for Surface Dynamics)

83259.	Wang, X.-G., and E.L. Sibert III, "A Nine-Dimensional Perturbative Treatment of the Vibrations of Methane and Its Isotopomers," *J. Chem. Phys.* 111, 4510-4522 (1999).	Vibrational Levels CH_4 Isotopomers Force Constants Calculations
83260.	Michaille, L., U. Rasbach and J.P. Pique, "Regularity of the Vibrational Spectrum of the CS_2 in the Σ_g^+ State: Our Previous Results Revisited," *J. Chem. Phys.* 111, 2968-2972 (1999).	Vibrational Energy Levels CS_2(X) Spectral Regularity $\leq$18,000 cm^{-1}
83261.	Di Lonardo, G., L. Fusina, E. Venuti, J.W.C. Johns, M.I. El Idrissi, J. Lievin and M. Herman, "The Vibrational Energy Pattern in Acetylene. V. $^{13}C_2H_2$," *J. Chem. Phys.* 111, 1008-1016 (1999).	Vibrational Energy Levels $^{13}C_2H_2$(X) $\leq$23670 cm^{-1} Data Analysis Assignments
83262.	Gremaud, B., D. Delande and N. Billy, "Highly Accurate Calculation of the Energy Levels of the H_2^+ Molecular Ion," *J. Phys. B. At. Mol. Opt. Phys.* 31, 383-392 (1998).	Vibrational Energy Levels H_2^+ Accurate Calculations
83263.	Varandas, A.J.C., H.G. Yu and Z.R. Xu, "Vibrational Spectrum of Ground State Li_3 and Statistical Analysis of the Energy Levels," *Mol. Phys.* 96, 1193-1206 (1999).	Vibrational Energy Levels Li_3 Calculations
83264.	Jongma, R.T., S. Shi and A.M. Wodtke, "Electronic Nonadiabaticity in Highly Vibrationally Excited $O_2(X^3\Sigma_g^-)$: Spin-Orbit Coupling between $X^3\Sigma_g^-$ and $b^1\Sigma_g^+$," *J. Chem. Phys.* 111, 2588-2594 (1999).	O_2(X,v=26-31) Term Values Constants O_2(X,v=28/b,v=19) Perturbation Analysis
83265.	Ma, G., and H. Guo, "Quantum Calculations of Highly Excited Vibrational Spectrum of Sulfur Dioxide. II. Normal to Local Mode Transition and Quantum Stochasticity," *J. Chem. Phys.* 111, 4032-4040 (1999).	Vibrational Energy Levels SO_2 $\leq$25,000 cm^{-1} Calculations

83266.	Duncan, A.H., and M.A. Collins, "Construction of Interpolated Potential Energy Surfaces Using Constrained Dynamics: Application to Rotational Inelastic Scattering," *J. Chem. Phys.* 111, 1346-1353 (1999).	P.E. Surfaces Interpolation Construction Method Testing
83267.	Hollebeek, T., T.-S. Ho and H. Rabitz, "Constructing Multidimensional Molecular Potential Energy Surfaces from ab Initio Data," *Ann. Rev. Phys. Chem.* 50, 537-570 (1999).	P.E. Surfaces Construction Methods CO.He OH(A).Ar $O(^1D) + H_2$ Review
(83296)	Polyatomics, Anharmonic Vibrational State Calculations, H_2O, $(H_2O)_2$ $Cl^-(H_2O)$	P.E. Surface Algorithm
83268.	Sohlberg, K., and D.R. Yarkony, "On the Strongly Bound $B^3\Pi$ State of the CAr van der Waals Complex: Bonding and Predissociation," *J. Chem. Phys.* 111, 3070-3076 (1999).	P.E. Curves $CAr(B,1^5\Sigma^-)$ Spin-Orbit Coupling Predissociation Rates D_e(B-State)
83269.	de Brouckere, G., and D. Feller, "Configuration Interaction Calculations on the $A^2\Pi_i$ State of CP and the $(A^2\Pi_i$-$X^2\Sigma^+)$ Transition Bands: Miscellaneous Properties," *J. Phys. B. At. Mol. Opt. Phys.* 31, 5053-5075 (1998).	P.E. Curves CP(A,X) Spectral Constants F.C. Factors Calculations
83270.	Brown, S.T., T.J. van Huis, B.C. Hoffman and H.F. Schaefer III, "Excited Electronic States of Carbon Disulfide," *Mol. Phys.* 96, 693-704 (1999).	P.E. Curves CS_2 7 Low-lying States Geometries Energies
(83355)	Isomers, P.E. Surfaces, PAs, Calculations	$C_2H_3F_2^+$ $C_2H_3Cl_2^+$
83271.	Moule, D.C., and E.C. Lim, "The Electronic Spectroscopy of Molecules Undergoing Large Amplitude Motions: Acetaldehyde in the First Excited Singlet and First Triplet States," pp. 110-134 in *Structure and Dynamics of Electronic Excited States*, J. Laane, H. Takahashi and A. Bandrauk, eds., 12 Papers Presented at the Pacifichem 95 Meeting, Held in Honolulu HI, December 1995, 320 pp., Springer-Verlag, Berlin (1999).	P.E. Surfaces $CH_3CHO(S_1,T_1)$ Jet Cooled LIF Torsion/Wagging Barriers
83272.	Blowers, P., and R.I. Masel, "An ab Initio Calculation of the Potential for the Interaction of a Hydrogen Atom with an Ethane Molecule," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7725-7729 (1999).	Interaction Potentials $C_2H_6 + H$ Calculations
(83125)	P.E. Surfaces, Channels, Energies, Dynamics	$C_3H_4 + h\nu$

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P.E. Surfaces
c-Ketones(S_1)
$(C_6H_5CH)_2$
Jet Cooled
LIF
Review

83274. Lin, S.Y., S.C. Park and M.S. Kim, "Construction of an Accurate Potential Energy Surface by Interpolation for Quantum Dynamics Studies of a Three-Body System," *J. Chem. Phys.* 111, 3787-3790 (1999).

P.E. Surface
$Cl+H_2$
Interpolation
Construction
Method

83275. Williams, J., A. Rohrbacher, J. Seong, N. Marianayagam, K.C. Janda, R. Burcl, M.M. Szczesniak, G. Chalasinski, S.M. Cybulski and N. Halberstadt, "A Three-Dimensional Potential Energy Surface for $He+Cl_2(B^3\Pi_{0u+})$: Ab Initio Calculations and a Multiproperty Fit," *J. Chem. Phys.* 111, 997-1007 (1999).

P.E. Surface
Cl_2(B,v)+He
Predissociation
Lifetimes
Product States
Calculations

83276. Sumathi, R., and S.D. Peyerimhoff, "Density Functional Characterization of [$HClO_2$] Potential Energy Surface," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7515-7521 (1999).

P.E. Surfaces
$HClO_2$
Isomers
Dissociation
Channels

83277. Ding, S., and Y. Zheng, "Lie Algebraic Approach to Potential Energy Surface for Symmetric Triatomic Molecules," *J. Chem. Phys.* 111, 4466-4471 (1999).

P.E. Surfaces
Triatomics
Algebraic
Approach
H_2O,H_2S

83278. Kuhn, B., T.R. Rizzo, D. Luckhaus, M. Quack and M.A. Suhm, "A New Six-Dimensional Analytical Potential up to Chemically Significant Energies for the Electronic Ground State of Hydrogen Peroxide," *J. Chem. Phys.* 111, 2565-2587 (1999).

P.E. Surface
H_2O_2
Properties
Calculations

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P.E. Surfaces
H_2S
Absorption
Spectrum
Photodissociation
Calculations

83280. Kleinekathofer, U., K.T. Tang, J.P. Toennies and C.L. Yiu, "The Generalized Heitler-London Theory for the H_3 Potential Energy Surface," *J. Chem. Phys.* 111, 3377-3386 (1999).

P.E. Surface
H_3
Calculation
General Theory

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P.E. Curve
Kr_2
Well Depth
Calculations

83282. Behmenburg, W., A. Kaiser, F. Rebentrost, M. Jungen, M. Smit, M. Luo and G. Peach, "Optical Transitions in Excited Alkali+Rare Gas Collision Molecules and Related Interatomic Potentials: Li*Ne," *J. Phys. B. At. Mol. Opt. Phys.* 31, 689-708 (1998).

P.E. Curves
LiNe
Optical
Transitions
Barrier Parameters
Calculations

83283. Zemke, W.T., and W.C. Stwalley, "Analysis of Exchange Energy at Long Range for States of Alkali Diatomic Molecules Correlating to Two Ground State Atoms," *J. Chem. Phys.* 111, 4962-4965 (1999).

P.E. Curves
Li_2,Na_2,K_2,NaK
Long Range
Exchange Energy
Formalism

83284. Linton, C., F. Martin, A.J. Ross, I. Russier, P. Crozet, A. Yiannopoulou, L. Li and A.M. Lyyra, "The High Lying Vibrational Levels and Dissociation Energy of the $a^3\Sigma_u^+$ State of $^7Li_2$," *J. Mol. Spectrosc.* 196, 20-28 (1999).

P.E. Curve
Li_2(a),v≤9
($2^3\Pi_g$-a)
OODR Spectrum
a-State Constants
D_0,Te

83285. Magnier, S., S. Rousseau, A.R. Allouche, G. Hadinger and M. Aubert-Frecon, "Potential Energy Curves of 58 States of Li_2^+," *Chem. Phys.* 246, 57-64 (1999).

P.E. Curves
Li_2^+
58 States
Spectral Constants
T_e,D_e

83286. Leung, A.W.K., R.R. Julian and W.H. Breckenridge, "Potential Curves for Several Electronic States of the MgHe, Mg^+He and Mg^{+2}He van der Waals Complexes," *J. Chem. Phys.* 111, 4999-5003 (1999).

P.E. Curves
MgHe,Mg^+He
van der Waals
Doubly Excited
States
Spectral Constants
D_e

83287. Rabadan, I., and J. Tennyson, "Erratum - Ab Initio Potential Energy Curves of Rydberg, Valence and Continuum States of NO [*J. Phys. B. At. Mol. Opt. Phys.* 30, 1975-1988 (1997)]," *ibid.* 31, 4485-4487 (1998).

P.E. Curves
NO
Erratum

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P.E. Curves
NaK(a,X)
Data Fitting
D_e(a,X)

83289.	Elbs, M., O. Keck, H. Knockel and E. Tiemann, "Long-Range Interactions in Molecules and Rotational Coupling," *Z. Phys. D. Atoms, Molecules, Clusters* 42, 49-55 (1997).	P.E. Curves Na_2 Long Range Asymptotic Structure
83290.	Liu, Y., J. Li, D. Chen, L. Li, K.M. Jones, B. Ji and R.J. Le Roy, "Molecular Constants and Rydberg-Klein-Rees (RKR) Potential Curve for the $Na_2(1^3\Sigma_g^-)$ State," *J. Chem. Phys.* 111, 3494-3497 (1999).	P.E. Curve $Na_2(1^3\Sigma_g^-)$ Band Constants $v \leq 57$ D_0
83291.	Yarkony, D.R., "Suppressing the Geometric Phase Effect: Closely Spaced Seams of the Conical Intersection in $Na_3(2^2E')$," *J. Chem. Phys.* 111, 4906-4912 (1999).	P.E. Surfaces $Na_3(2^2E')$ Conical Intersection Seam Calculations
(83010)	P.E. Surfaces, Cross Sections, Coupling Effects, Analysis	$O(^1D) + H_2$
(83011)	P.E. Surface, v = 0, J Dependence, Testing	$O(^1D) + n\text{-}H_2/p\text{-}H_2$
83292.	Morrill, J.S., M.L. Ginter, B.R. Lewis and S.T. Gibson, "The $(X^2\Pi_g)ns\sigma_g\,^{1,3}\Pi_g$ Rydberg States of O_2: Spectra, Structures and Interactions," *J. Chem. Phys.* 111, 173-185 (1999).	P.E. Curves $O_2(^{1,3}\Pi_g)$ Rydberg/Valence 6.5-9.5 eV Predissociations Assignments
83293.	Turski, P., and M. Barysz, "Electronic States of the Copper Silicide and Its Ions," *J. Chem. Phys.* 111, 2973-2977 (1999).	P.E. Curves $SiCu, SiCu^{\pm}$ Low-lying States Spectral Constants D_e Calculations
83294.	Jimeno, P., M.D. Gray and G.G. Balint-Kurti, "Ab Initio Potential Energy Surface for the Ground ($^2A'$) State of H + SiO and Rotationally Inelastic Collision Cross Sections for Circumstellar H + SiO Collisions," *J. Chem. Phys.* 111, 4966-4975 (1999).	P.E. Surface SiO/H v,J Energy Transfer Calculations
83295.	Cai, Z.-L., and J.P. Francois, "Ab Initio Study of the Electronic Spectrum of the SiO^+ Cation," *J. Mol. Spectrosc.* 197, 12-18 (1999).	P.E. Curves SiO^+ Low-lying States Spectral Constants D_e ,T_e Lifetimes Calculations

44. ATOMIC/MOLECULAR STRUCTURES

(See also Section 26 for Spectrally Measured Structures)

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83297.	Watson, J.K.G., A. Roytburg and W. Ulrich, "Least-Squares Mass-Dependence Molecular Structures," *J. Mol. Spectrosc.* 196, 102-119 (1999).	Molecular Structures Polyatomics Spectral Analysis Difficulties HCN,H_2O,H_2S OCS,Hydrides
83298.	Baeck, K.K., H. Choi and S. Iwata, "Theoretical Study on Spectroscopic Properties of Positive, Neutral and Negative Species of BCl_2 and $AlCl_2$: The Stability of the Negative Species," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6772-6777 (1999).	Structural Calculations $BCl_2,AlCl_2$ $BCl_2^+,AlCl_2^+$ $BCl_2^-(a,X),AlCl_2^-(a,X)$ Geometries Frequencies IP,EA S/T Energy Splitting
83299.	Flowers, B.A., and J.S. Francisco, "A Coupled-Cluster Study of the Molecular Structure, Vibrational Frequencies and Energetics of $COBr^+$ and $BrCO^+$ Cations," *J. Chem. Phys.* 111, 3464-3467 (1999).	Structural Calculations $BrCO^+,COBr^+$ Geometries Frequencies D
83300.	Hu, C.-H., "A Comparative Study of the Singlet-Triplet Energy Separation of Carbenes Using Density Functional Theory and Coupled-Cluster Methods," *Chem. Phys. Lett.* 309, 81-89 (1999).	Structural Calculations ^{1,3}Energy Splitting $CF_2,CFCl,CCl_2$ CH_2,CHF,CHCl $CH_3CH,CHNO_2,C(CH_3)_2$
83301.	Margules, L., J. Demaison and J.E. Boggs, "Equilibrium C-F Bond Length and Structure of Formyl Fluoride, Difluorocarbene, Monofluoromethylene and Difluoromethane," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7632-7638 (1999).	Structural Calculations CF_2,CHF CH_2F_2,CHFO Geometries

83302.	Francisco, J.S., "Coupled Cluster Study of the Structure and Vibrational Spectrum of $HC(O)O^+$," *Mol. Phys.* 96, 877-880 (1999).	Structural Calculations $HC(O)O^+$ Geometry Frequencies
83303.	Schwartz, M., and P. Marshall, "An ab Initio Investigation of Halocarbenes," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7900-7906 (1999).	Structural Calculations CH_2,CHX CX_2,CXY X,Y=Halogen Geometries Frequencies ^{1,3}Energy Splittings
83304.	Francisco, J.S., "An ab Initio Study of the Structures and Energetics of CH_3OCl and CH_3ClO," *Int. J. Quantum Chem.* 73, 29-35 (1999).	Structural Calculations CH_3OCl CH_3ClO Geometries Frequencies ΔH_f
83305.	Suzuki, Y.-I., "Structure of Molecular Energy Levels of Homonuclear Diatomic Molecules," *Int. J. Quantum Chem.* 72, 597-604 (1999).	Electronic Structures C_2,C_2^+ Sc_2,Ti_2 Low-lying States Bond Order Predictive Method
83306.	Ihee, H., A.H. Zewail and W.A. Goddard III, "Conformations and Barriers of Haloethyl Radicals (CH_2XCH_2, X=F,Cl,Br,I): Ab Initio Studies," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6638-6649 (1999).	Structural Calculations CH_2XCH_2 X=F,Cl,Br,I Geometries Frequencies Energies
83307.	Christiansen, O., J. Gauss, J.F. Stanton and P. Jorgensen, "The Electronic Spectrum of Pyrrole," *J. Chem. Phys.* 111, 525-537 (1999).	Structural Calculations *c*-C_4H_5N Low-lying States Geometries Frequencies Oscillator Strengths Energies
83308.	Godfrey, P.D., R.N. Jorissen and R.D. Brown, "Shapes of Molecules by Millimeter-Wave Spectroscopy: 2-Phenylethanol," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7621-7626 (1999).	Structure $C_6H_5CH_2CH_2OH$ Microwave Spectrum

83309. Chien, S.-H., K.-C. Lau, W.-K. Li and C.Y. Ng, "Energetics and Structures of the Carbonyl Chloride Radical, Oxalyl Chloride and Their Cations," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7918-7922 (1999).

Structural Calculations
$ClCO, ClCO^+$
$(ClCO)_2, (ClCO)_2^+$
Geometries
ΔH_f, IP(ClCO)

83310. Deng, K., J. Yang, L. Yuan and Q. Zhu, "A Theoretical Study of the Linear OCuO Species," *J. Chem. Phys.* 111, 1477-1482 (1999).

Structural Calculations
$CuO_2, CuO_2^{\pm}$
Linear Geometry
Frequencies
PES Spectrum

83311. Guha, S., and J.S. Francisco, "An Examination of the Reaction Pathways for the HOOOBr and HOOBrO Complexes Formed from the HO_2+BrO Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 8000-8007 (1999).

Structural Calculations
$HBrO_3$
Isomers
Geometries
Frequencies
HO_2+BrO
Dynamics

83312. Yamaguchi, Y., B.C. Hoffman, J.C. Stephens and H.F. Schaefer III, "Three Lowest-lying Electronic States of NH_2," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7701-7708 (1999).

Electronic Structural Calculations
NH_2(B,A,X)
Energies
Geometries
Frequencies
IR Intensities

83313. Xie, Y., H.F. Schaefer III, X.-Y. Fu and R.-Z. Liu, "The Infrared Spectrum of the Nitric Oxide Dimer Cation: Problems for Density Functional Theory and a Muddled Relationship to Experiment," *J. Chem. Phys.* 111, 2532-2541 (1999).

Structural Calculations
$(NO)_2^+$
Geometries
Frequencies
IR Intensities

(83368) Structural Calculations, D, EAs — SeF_n, n=1-7

83314. Brown, S.T., Y. Yamaguchi and H.F. Schaefer III, "The Disilaketenyl Radical (HSiSiO) in Its Ground and First Excited Electronic States," *J. Chem. Phys.* 111, 227-234 (1999).

Structural Calculations
HSiSiO(A,X)
Geometries
Frequencies
IR Intensities
Dipole Moments

83315. Xie, D., X. Xu, Y. Xue and G. Yan, "Density Functional Theory Studies on Vibrational Spectra of Si_2H_5X (X=F,Cl,Br) and Their Isotopomers," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 7437-7444 (1999).

Structural Calculations
Si_2H_5X
X=F,Cl,Br
Geometries
Frequencies

45. ENERGY TRANSFER

(See also Section 27 for Electronically Excited State Relaxation Processes)

83316. Suzuki, T., L. Wang and H. Kohguchi, "Femtosecond Time-Resolved Photoelectron Imaging on Ultrafast Electronic Dephasing in an Isolated Molecule," *J. Chem. Phys.* 111, 4859-4861 (1999).

Electronic Relaxation
c-$C_4H_4N_2(S_1/T)$
fs Photoelectron Visualization

(83112) Relaxation Rates, Measurements

CF_3(T,v)+Ar

83317. Coletti, C., and G.D. Billing, "Isotopic Effects on Vibrational Energy Transfer in CO," *J. Chem. Phys.* 111, 3891-3897 (1999).

Vibrational Energy Transfer
CO(v=1)+$^{13}C^{18}O$
CO(v=1)+^{13}CO
CO(v=1)+CO
Rate Constant Calculations

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(82960)	$NO^+(a, v=0\text{-}16)\text{-}NO(X)$,PFI/PES Spectrum	IP(NO)
(83288)	P.E. Curves, Data Fitting	$D_e(NaK(a,X))$
(83290)	P.E. Curve, v≤57, Band Constants, Analysis	$D_0(Na_2(1^3\Sigma_g^-))$
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